

chain nodes :
6 7 8 10 11
ring nodes :
1 2 3 4 5
chain bonds :
1-10 6-7 6-8 7-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:Atom

Generic attributes :

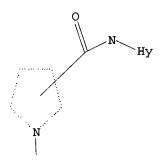
11:

Number of Carbon Atoms : less than 7 Number of Hetero Atoms : less than 2 Type of Ring System : Monocyclic

Element Count : Node 11: Limited C,C4 S,S1

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 11:59:12 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 87815 TO ITERATE

2.3% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS:

1738707 TO 1773893

PROJECTED ANSWERS:

0 TO (

L2

0 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 11:59:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 753988 TO ITERATE

41.1% PROCESSED 720923 ITERATIONS

310 ANSWERS

0 ANSWERS

51.4% PROCESSED 902313 ITERATIONS

316 ANSWERS

55.8% PROCESSED 978997 ITERATIONS

316 ANSWERS

57.0% PROCESSED 1000000 ITERATIONS

316 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.52

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS:

1753988 TO 1753988

624

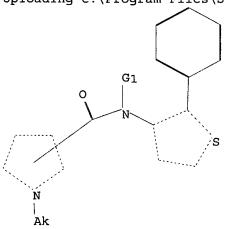
PROJECTED ANSWERS:

484 TO

L3 316 SEA SSS FUL L1

=>

Uploading C:\Program Files\Stnexp\Queries\10680346B.str



20 22 19 23 16 18 18 10 10 23 15 14

chain nodes : 6 7 8 10 16 ring nodes :

1 2 3 4 5 11 12 13 14 15 18 19 20 21 22 23

chain bonds :

1-10 6-7 6-8 7-11 7-16 12-18

ring bonds :

1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15 18-19 18-23 19-20 20-21

21-22 22-23

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-16 11-12 11-15 12-13 13-14 14-15

exact bonds :

12-18

normalized bonds :

18-19 18-23 19-20 20-21 21-22 22-23

G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:CLASS 13:Atom 14:Atom 15:Atom 16:CLASS 18:Atom 19:Atom 20:Atom

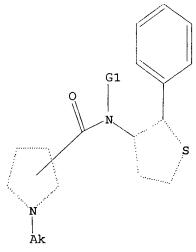
21:Atom 22:Atom 23:Atom

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR



G1 H, Me

Structure attributes must be viewed using STN Express query preparation.

=> s 14

SAMPLE SEARCH INITIATED 12:03:05 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 15 TO ITERATE

100.0% PROCESSED 15

15 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 68 TO 532 PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s 14 full

FULL SEARCH INITIATED 12:03:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 469 TO ITERATE

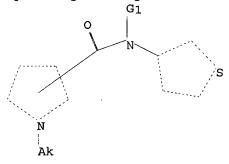
100.0% PROCESSED 469 ITERATIONS 6 ANSWERS

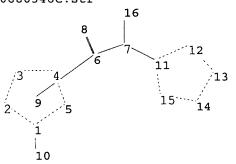
SEARCH TIME: 00.00.01

L6 6 SEA SSS FUL L4

=>

Uploading C:\Program Files\Stnexp\Queries\10680346C.str





chain nodes : 6 7 8 10 16 ring nodes :

1 2 3 4 5 11 12 13 14 15

chain bonds :

1-10 6-7 6-8 7-11 7-16

ring bonds :

1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-16 11-12 11-15 12-13 13-14 14-15

G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:CLASS 13:Atom 14:Atom 15:Atom 16:CLASS

L7 STRUCTURE UPLOADED

=> s 17

SAMPLE SEARCH INITIATED 12:04:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 940 TO ITERATE

100.0% PROCESSED 940 ITERATIONS 11 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

Page 630/08/2005

PROJECTED ITERATIONS: 16961 TO 20639 PROJECTED ANSWERS: 22 TO 418

L8 11 SEA SSS SAM L7

=> s 17 full

FULL SEARCH INITIATED 12:04:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 17912 TO ITERATE

100.0% PROCESSED 17912 ITERATIONS 243 ANSWERS

SEARCH TIME: 00.00.01

L9 243 SEA SSS FUL L7

=> fil caplus

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 487.43 487.64

FILE 'CAPLUS' ENTERED AT 12:05:19 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 19

L10 22 L9

=> d ed abs ibib hitstr 110

ANSWER 1 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 07 Apr 2005

The invention relates to quinazoline derivs. I {R2 or the substituted pyrrolidinyloxy group is in the 6 or 7 position of the quinazoline ring: A is Ph or pyridyl; m is 0-3; n is 0-2; R1 is halo, cyano, nitro, hydroxy, carboxy, trifluoromethyl, alkyl, alkoxy, alkylsulfonyl, alkylureido, etc.: R2 is H, alkyl, cycloalkyl, cycloalkyl alkylureido; carbamylalkyl, cycloalkyl, alkylthio, alkylsulfinyl, carbamylalkyl, etc.: R4 is alkyl, alkoxy, cyano, halo, hydroxy or oxo: R5 is H or alkyl: R6 is H, alkyl, alkoxy, beterocyclyl, heteroaryl, etc.: or R5K6N is a ringl, including processes for their preparation, pharmaceutical compns. containing

, and their use as antiproliferative agents in the prevention or treatment of tumors which are sensitive to inhibition of erbB receptor tyrosine kinases. Thus, compound II was prepared by etherification of Boc-protected cis-4-hydroxy-D-proline Me ester with 4-chloro-7-methoxyquinazolin-6-ol and reaction of the product with 3-chloro-2-fluoroannilne in 4.0 M HCI/dioxane and acetonitrile, followed by reductive N-methylation, nification.

HCI/dioxane and acetonitrile, followed by requestive notation, and amidation. Compound II showed IC50 = 0.008 nM for inhibition of EGFR tyrosine kinase protein phosphorylation and IC50 = 0.144 nM in the EGFR driven KB cell proliferation assay.

ACCESSION NUMBER: 2005:300434 CAPLUS
DOCUMENT NUMBER: 142:374111

TITLE: Preparation of proline quinazoline derivatives as antiproliferative agents
INVENTOR(S): Bradbury, Robert Hugh; Halsall, Christopher Thomas: Hennequin, Laurent Francois Andre; Kettle, Jason Grant; Plowright, Alleyn

L10 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)
PATENT ASSIGNEE(S):
SOURCE:
PCT Int. Appl., 198 pp.
CODEN: PIXXD2

DOCUMENT TYPE:
Patent
Follows:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: English 2

NO. KIND DATE APPLICATION NO. DATE

5030757 A1 20050407 M0 2004-GB4085 M, BZ 20040922
AE, AG, AL, AH, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CC, CG, CR, CU, CZ, DE, DK, DH, DZ, EC, EZ, EG, ES, F1, GB, GD, GE, GH, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, DM, MG, KK, MM, MW, KK, MZ, NA, IN, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TM, TT, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZM, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AE, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CT, CZ, DE, DK, EE, ES, F1, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SN, TD, TG

LIN. INFO:: PATENT NO. WO 2005030757

GB 2003-22409 GB 2003-22534 PRIORITY APPLN. INFO.: A 20030925 A 20030926

OTHER SOURCE(S): IT 849345-53-5P MARPAT 142:374111

RE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of proline quinazoline derivs. as antiproliferative agents) 849345-53-5 CAPLUS

2-Pyrrolidinecarboxamide, 4-[[4-((3-chloro-2-fluorophenyl)amino]-7-methoxy-6-quinazolinyl)oxy]-1-methyl-N-3-thienyl-, (2R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ed abs ibib hitstr 1-22

ANSWER 1 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 07 Apr 2005

The invention relates to quinazoline derivs. I [R2 or the substituted pyrrolidinyloxy group is in the 6 or 7 position of the quinazoline ring; A is Ph or pyridyl: m is 0-3; n is 0-2; R1 is halo, cyano, nitro, hydroxy, carboxy, trifluoromethyl, alkyl, alkoxy, alkylsulfonyl, alkylureido, etc.; R2 is H, alkyl, cycloalkyl, cycloalkylalkyl or (un)substituted alkoxy; R3 is H, alkyl, cycloalkyl, skylthio, alkylsulfinyl, carbamoylalkyl, etc.; R4 is alkyl, alkoxy, cyano, halo, hydroxy or oxo; R5 is H or alkyl; R6 is H, alkyl, alkoxy, heterocyclyl, heteroaryl, etc.; or R5R6N is a ringl, including processes for their preparation, pharmaceutical compns. containir,

and their use as antiproliferative agents in the prevention or treatment of tumors which are sensitive to inhibition of erbB receptor tyrosine kinases. Thus, compound II was prepared by etherification of Boc-protected cis-4-hydroxy-D-proline Me eater with 4-chloro-7-methoxyquinazolin-6-ol and reaction of the product with 3-chloro-2-fluoroanniline in 4.0 M HCl/dioxane and acetonitrile, followed by reductive N-methylation, inification. saponification.

nification, Compound II showed IC50 = 0.008 nM for inhibition of EGFR tyrosine kinase protein phosphorylation and IC50 = 0.144 nM in the EGFR driven KB cell proliferation assay.

SION NUMBER: 2005:300434 CAPLUS

MENT NUMBER: 142:374111

ACCESSION NUMBER:

DOCUMENT NUMBER: TITLE:

Preparation of proline quinazoline derivatives as antiproliferative agents Bradbury, Robert Hugh; Halsall, Christopher Thomas; Hennequin, Laurent Francois Andre; Kettle, Jason Grant: Plowright, Billiam . INVENTOR(S):

Grant; Plowright, Alleyn

ANSWER 2 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 24 Sep 2004 L10

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

DOCUMENT NUMBER: 141:295864

Preparation of sulfonamide lactams as Factor Xa inhibitors O'Connor, Stephen P.; Lawrence, Michael; Shi, Yan; Stein, Philip D.

INVENTOR(S):

USA
U.S. Pat. Appl. Publ., 257 pp.
CODEN: USXXCO
Patent PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE A1 US 2004186134 20040923 US 2003-374299 20030226 PRIORITY APPLN. INFO.: OTHER SOURCE(S): IT 445277-00-9P US 2003-374299 MARPAT 141:295864

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(drug candidate; preparation of sulfonamide lactams as factor Xa inhibitors and anticoagulants)
445277-00-9 CAPLUS
2-Pyrrolidinecarboxamide, 1-[(3S)-3-[[(1E)-2-(5-chloro-2-thleny)]sulfony]jamino]-2-oxo-1-piperidiny]jacety]}-N-(tetrahydro-1,1-dioxido-3-thleny])-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

L10 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continu PATEMT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Ltd. SOURCE: CODEN: PIXXD2

DOCUMENT TYPE: EARGUAGE: Facent English FAMILY ACC. NUM. COUNT: 2 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE WO 2005030757 A1 20050407 WO 2004-GB4085 20040922 0.30757 A1 20050407 W0 2004-GB4085 20040922
AE. AG, AL. AM, AT. AU. AZ. BB. BB. BG, BR. BW, BY, BZ. CA. CL. CN. CO. CR. CU, CZ. DE. DK, DM, DZ. EC. EE, EG. ES, FI. GB, GD. GE, GH, GM, HR, HU, ID. II., IN. IS. JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MK, MZ, NR, NI, NO. NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TH, TN, TT, TT, TZ, UA, UG, US, UZ, VC, VN, VU, ZA, ZH, ZW, BW, GH, GM, KE, LS, MW, MZ, NR, AD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, NG, EE, ES, FI. FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, RT, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG GE, LK, NO, TJ. RW: BW, AZ, EE, SI,

GB 2003-22409 GB 2003-22534 PRIORITY APPLN. INFO.: A 20030925 A 20030926

OTHER SOURCE(S): MARPAT 142:374111

IT 849345-53-5P

RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of proline quinazoline derivs. as antiproliferative agents) 849345-53-5 CAPLUS 2-Pyrrolidinecarboxamide, 4-[[4-[(3-chloro-2-fluorophenyl)amino]-7-methoxy-6-quinazolinyl]oxy]-1-methyl-N-3-thienyl-, (2R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT REFERENCE COUNT:

L10 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 13 May 2004

A fungicidally active compound I, II, or III [wherein Het = (un)substituted 5- or 6-membered heterocyclic ring containing one to three O, N, and/or S atoms, provided that the ring is not 1,2,3-triazole: R1 and R2 = independently H, halo, or Me: R3 = (un)substituted (cyclo)alkyl, alkenyl, alkenyl, Ph, heterocyclyl: R7 and R8 = independently H, halo, or (halo)alkyl] were prepared for use as active ingreddents in agricultural or hotticultural compns. for controlling or preventing infestation of plants by phytopathogenic microorganisms, preferably fungi. For example, 3-difluoromethyl-1-methyl-1H-pyrazole-4-carboxylic acid was amidated with [2-(bicyclopropyl-2-yl)thiophen-3-yl]amine in the presence of TEA and N,N-bis(2-oxooxazolidinyl)phosphinic acid chloride in CH2Cl2 to give trans-IV [978 purity]. The latter showed excellent activity against Puccinia recondita on wheat (0-5% infestation) and showed good activity against Podosphaera leucotricha on apple, Venturia inaequalis on apple, Frysiphe graminis on barley, Pyrenophora teres on barley, Alternaria solani on tomato, and Uncinula necator on grape (<20% infestation for each).

each).
ACCESSION NUMBER: 2004:390242 CAPLUS DOCUMENT NUMBER:

Preparation of N-(cyclopropylthienyl)carboxamides as

Engireund, Josef; Tobler, Hans; Walter, Harald Syngenta Participations Ag, Switz. PCT Int. Appl., 43 pp. CODEN: PIXXD2 INVENTOR (S):

PATENT ASSIGNEE (S):

SOURCE:

L10	ANSWER	3 OF	22 CAPLUS	COPYRIGH	T 2005 ACS	on STN	(Continued)
	688325-	-83-9P	688325-84	OP 688325-	35-1P		,
	688325-	-B6-2P	688325-87	-3P 688325-0	8-4P		
	688325-	-89-SP	688325-90	-BP 688325-	1-92		
	688325-	-92-0P	688325-93	-1P 688325-1	4-2P		
	688325	-95-3P	688325-96	-4P 688325-	7-5P		
	688325	-98-6P	688325-00	-7P 688326-	10-3P		
				-5P 688326-0			
				-BP 688326-			
				-1P 608326-			
				-6P 688326-			
				-OP 688326-			
				-3P 608326-			
				-BP 688326-2			
				-1P 688326-2			
				-4P 688326-2			
				-9P 688326-3			
				-2P 688326-			
				-SP 688326-			
				-SP 688326			
				-SP 688328-2	23-6P		
	688328-						
							unclassified). CD

(Synthetic preparation): BIOL (Biological study): PREP (Preparation): USES

(Sues) (fungicide; prepn. of N-(cyclopropylthienyl)carboxamides as fungicides) 688322-46-5 CAPLUS
H-Pyrrole-3-carboxamide, N-[2-(2-ethylcyclopropyl)-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-47-6 CAPLUS
1H-Pyrrole-3-carboxamide, N-{2-{2-ethylcyclopropyl}-3-thienyl}-1-(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-48-7 CAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[2-(2-propylcyclopropyl)-3-thienyl]-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS ON STN
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1 '(Continued)

PATENT NO KIND DATE APPLICATION NO. DATE 2004033799 A1 20040513 W0 2003-EP11805 20031024
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BB, BB, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, ILL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, NM, MM, MX, MZ, NI, NO, NZ, CM, EG, GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, SF, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, DF, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
2501739 AA 20040513 CA 2003-2501739 20031024
BISSORT A1 20050727 EP 2003-776869 20031024
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
APPLN. INFO:

MARPAT 140:406731 WO 2004039799 KW: GH, KG, FI, BF, CA 2501739 EP 1556377 PRIORITY APPLN. INFO.:

PRIORITY APPLN. INFO.:

OTHER SOURCE(S):

NARPAT 140:406731

IT 689322-46-5P 669322-47-6P 689322-46-7P 689322-49-8P 669322-55-1P 689322-55-2P 689322-55-4P 689322-55-5P 689322-55-5P 689322-55-5P 689322-55-6P 689322-55-6P 689322-56-5P 689322-56-5P 689322-56-5P 689322-56-6P 689322-66-9P 689322-66-9P 689322-66-9P 689322-67-0P 689322-67-0P 689322-67-0P 689322-77-2P 689322-73-8P 689322-86-3P 689322-96-5P 689323-06-5P 689323-06-5P 689323-06-5P 689323-06-5P 689323-1-1-P 689323

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

688322-49-8 CAPLUS
1H-Pyrrole-3-carboxamide, 4-{difluoromethyl}-1-methyl-N-{2-{2-propylcyclopropyl}-3-thienyl}- (9CI) (CA INDEX NAME)

688322-50-1 CAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[2-[2-(1-methylethyl)cyclopropyl]-3thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-51-2 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[2-{2-(1-methylethyl)cyclopropyl}-3-thienyl]- (9CI) (CA INDEX NAME)

688322-52-3 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-{2-[2-(1-methylethyl)cyclopropyl)-3-thienyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

1-Pr.

RN 688322-53-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[2-[2-(1-methylethyl)cyclopropyl]-3-thienyl]- (9C1) (CA INDEX NAME)

1-Pr 0 || C-NH

RN 688322-54-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1-ethyl-4-methyl-N-[2-[2-[1-methylethyl]cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

i-Pr O C-NH

RN 688322-55-6 CAPLUS
CN 1H-Fyrrole-3-carboxamide, 2-fluoro-1, 4-dimethyl-N-[2-[2-[1methylethyllcyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued

Ne N C-NH S

RN 688322-59-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-(2-butylcyclopropyl)-3-thienyl)-4(difluoromethyl)-1-methyl- (9Cf) (CA INDEX NAME)

Me N C-NH S

RN 688322-60-3 CAPLUS
CN lH-Pyrcole-3-carboxamide, N-[2-(2-butylcyclopropyl)-3-thienyl]-2-fluoro1.4-dimethyl- (9C1) (CA INDEX NAME)

Me O C-NH-S

RN 688322-61-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-butylcyclopropyl)-3-thienyl]-2-chloro1,4-dimethyl (9C1) (CA INDEX NAME)

n-Bu

N- 0

C- NH - S

RN 688322-62-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-{2-[2-[2-methylpropyl]cyclopropyl]-3-

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L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688322-56-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-ethyl-2-fluoro-4-methyl-N-[2-{2-{1-methyl-tyl-pyclopropyl}-3-thienyl}- (9CI) (CA INDEX NAME)

Me O C-NH

RN 688322-57-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-[chlorodifluoromethyl]-2-fluoro-1-methyl-N-[2-[2-(1-methylethyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

C1-CF2 O | C-NH-S

RN 688322-58-9 CAPLUS
CN IH-Fyrrole-3-carboxamide, N-(2-(2-butylcyclopropyl)-3-thienyl]-1-methyl-4(trifluoromethyl)- (SCI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688322-63-6 CAPLUS
CN 1H-Fyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[2-[2-(2-methylpropyl)-yclopropyl]-3-thienyl]- (9Ci) (CA INDEX NAME)

1-Bu

RN 688322-64-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-{fluoromethyl}-1-methyl-N-{2-{2-(2-methylpropyl)cyclopropyl}-3-thienyl}- (9CI) (CA INDEX NAME)

i-Bu
O
C-NH
S

RN 688322-65-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(methoxymethyl)-N-[2-[2-(2-methylpropyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

1-BU
O
C-NH
CF3

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688322-66-9 CAPLUS
1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-{2-{2-{2-methylpropyl}cyclopropyl}-3-thienyl}- (9CI) (CA INDEX NAME)

688322-67-0 CAPLUS
1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[2-[2-{2-methylpropyl}cyclopropyl}-3-thienyl]- (9CI) (CA INDEX NAME)

688322-68-1 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-[2-(1,1-dimethylethyl)cyclopropyl]-3thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-69-2 CAPLUS IH-Pyrrole-3-carboxamide, 4-(difluoromethyl)-N-(2-[2-(1,1-dimethyl-thyl)cyclopropyl)-3-thienyl)-1-methyl- (9C1) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

688322-73-8 CAPLUS IH-Pyrrole-3-carboxamide, 1-methyl-N-[2-(2-pentylcyclopropyl)-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-74-9 CAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-{2-[2-(3-methylbutyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- {9Cl} (CA INDEX NAME)

688322-75-0 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[2-[2-(3-methylbutyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

688322-76-1 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-{2-hexylcyclopropy1}-3-thieny1}-1-methyl-4-

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L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688322-70-5 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-[2-(1,1-dimethylethyl)cyclopropyl]-3-thienyl]-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

688322-71-6 CAPLUS
1H-Pyrrole-3-carboxamide, 2-chloro-N-(2-[2-(1,1-dimethylethyl)cyclopropyl]-3-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

68832-72-7 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-(2-(2-(1,1-dimethylethyl)cyclopropyl)-3-thienyl)-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-77-2 CAPLUS
1H-Pyrrole-3-carboxamide, N-(2-[1,1'-bicyclopropy1]-2-y1-3-thieny1)-1-methy1-4-(trifluoromethy1)- (9C1) (CA INDEX NAME)

688322-78-3 CAPLUS 1H-Pyrrole-3-carboxamide, N-(2-(1,1'-bicyclopropyl)-2-yl-3-thienyl)-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

688322-79-4 CAPLUS
1H-Pyrrole-3-carboxamide, N-(2-[1,1'-bicyclopropyl]-2-yl-3-thienyl)-2-fluoro-1,4-dimethyl- (9Cl) (CA INDEX NAME)

688322-80-7 CAPLUS
1H-Pyrrole-3-carboxamide, N-{2-{1,1'-bicyclopropyl}-2-yl-3-thienyl}-2-chloro-1,4-dimethyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me O C-NH-S

RN 688322-81-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-(2-cyclobutylcyclopropyl}-3-thienyl}-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me C-NH CF3

RN 688322-82-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cyclobutylcyclopropyl)-3-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

Me N C-NH S

RN 688322-83-0 CAPLUS
CN 1H-Fyrrole-3-carboxamide, N-{2-(2-cyclopentylcyclopropyl)-3-thienyl}-1methyl-4-{trifluromethyl)- (9C1) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continue

RN 688322-86-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-(2-(2-cyclopentylcyclopropyl)-3-thienyl)-1-methyl- (9CI) (CA INDEX NAME)

C1- CF2 C=0

RN 688322-87-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cyclopentylcyclopropyl)-3-thienyl]-2-fluorol, 4-dimethyl- (9C1) (CA INDEX NAME)

Me C O

RN 688322-88-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-N-[2-(2-cyclopentylcyclopropyl)-3-thienyl]-1,4-dimethyl- (9C1) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

F₃c C C NH

RN 688322-84-1 CAPLUS
CN 1H-Pyrcole-3-carboxamide, N-[2-(2-cyclopentylcyclopropyl)-3-thienyl]-4(diflucromethyl)-1-methyl- (9CI) (CA INDEX NAME)

F₂CH C= C

RN 688322-85-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cyclopentylcyclopropyl)-3-thienyl]-4(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

FCH2 C

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me COOK

RN 688322-89-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-(2-cyclohexylcyclopropyl)-3-thienyl}-1-methyl-4-(trifluoromethyl)- {9CI} (CA INDEX NAME)

Me N CF3

RN 688322-90-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-(2-cyclohexylcyclopropyl)-3-thienyl}-4(diffuoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

Me CHF2

RN 688322-91-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cyclohexylcyclopropyl)-3-thienyl]-4(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

LIO ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me N C NH S

RN 688322-92-1 CAPLUS
CN 1H-Pycrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[2-(2-cyclohexylcyclopropyl)-3-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

Me N C-NH S

RN 688322-93-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-(3-cyclohexyl-2,2-difluorocyclopropyl)-3-thienyl}-1-methyl-4-{trifluoromethyl}- (9CI) (CA INDEX NAME)

Me C-NH S

RN 688322-94-3 CAPLUS
CN H-Fyrrole-3-carboxamide, N-[2-(2-cyclohexylcyclopropyl)-3-thienyl]-2fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continue

RN 688322-98-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cycloheptylcyclopropyl)-3-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688322-99-8 CAPLUS
CN HH-Pyrrole-3-carboxamide, N-[2-(2-cycloheptylcyclopropyl)-3-thienyl]-4(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688323-00-4 CAPLUS
CN IN-Fyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-(2-(2cycloheptylcyclopropyl)-3-thienyl)-1-methyl- (9C1) (CA INDEX NAME)

RN 688323-01-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-(2-cycloheptylcyclopropyl)-3-thienyl]-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688322-95-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-N-{2-(2-cyclohexylcyclopropyl)-3-thienyl}-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688322-96-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cycloheptylcyclopropyl)-3-thienyl]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688322-97-6 CAPLUS
CN 1H-Pytrole-3-carboxamide, N-[2-{2-cycloheptylcyclopropyl}-3-thienyl}-1-ethyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Cont.

RN 688323-02-6 CAPLUS
CN 1H-Pytrole-3-carboxamide, 2-chloro-N-[Z-(2-cycloheptylcyclopropyl)-3-thlenyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688323-03-7 CAPLUS
CN IH-Pyrrole-3-carboxamide, N-{2-(2-cyclooctylcyclopropyl)-3-thienyl}-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688323-04-8 CAPLUS
CN | H-Pyrrole-3-carboxamide, N-[2-(2-cyclooctylcyclopropyl)-3-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688323-05-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-{2-(2-phenylcyclopropyl)-3-thienyl}-4-

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) (trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688323-06-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[2-(2-phenylcyclopropyl)-3-thienyl]- (9CI) (CA INDEX NAME)

RN 688323-07-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-[2-(2-phenylcyclopropyl)-3-thienyl]- (9CI) (CA INDEX NAME)

RN 688323-08-2 CAPLUS
CN IM-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-[2-(2-phenylcyclopropyl)-3-thienyl]- (9Cl IMDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688323-12-6 CAPLUS
CN IH-Pyrrole-3-carboxamide, N-{2-[2-(4-chlorophenyl)cyclopropyl]-3-thienyl]1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688323-13-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-[2-(4-chlorophenyl)cyclopropyl]-3-thienyl]4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688323-14-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-[2-[4-bromophenyl]cyclopropyl]-3-thienyl}-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688323-09-3 CAPLUS
CN 1H-Pytrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[2-(2-phenylcyclopropyl)-3-thienyl]- (9C1) (CA INDEX NAME)

RN 688323-10-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-[2-(4-fluorophenyl)cyclopropyl}-3-thienyl]1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688323-11-7 CAPLUS
CN IH-Fyrrole-3-carboxamide, 4-(difluoromethyl)-N-[2-(2-(4-fluorophenyl)cyclopropyl)-3-thienyl)-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688323-15-1 CAPLUS
CN 1H-Fyrrole-3-carboxamide, N-[2-[2-(4-bromopheny1)cyclopropy1]-3-thieny1]-4(difluoromethy1)-1-methy1- (9CI) (CA INDEX NAME)

RN 688323-16-2 CAPLUS
CN H-Pyrcle-3-carboxamide, 1-methyl-N-[2-[2-(2-thienyl)cyclopropyl]-3-thienyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688323-17-3 CAPLUS
CN 1H-Pyrcole-3-carboxamide, 1-methyl-N-[2-[2-(3-thienyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

F3C S ONH

RN 688323-18-4 CAPLUS
CN H-Pyrrole-3-carboxamide, N-[2-[2-(2-furanyl)cyclopropyl]-3-thienyl]-1methyl-4-(trifluoromethyl)- (9C1) (CA INDEX NAME)

F3C C C

RN 688323-19-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-[2-(3-furany1)cyclopropy1]-3-thieny1]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

F3C C ON NH

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me O C-NH S

RN 688325-61-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-(2-ethylcyclopropyl)-3-thienyl]-1-methyl-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me N C-NH S

RN 688325-62-4 CAPLUS
CN 1H-Fyrrole-3-carboxamide, N-[4-(2-ethylcyclopropyl)-3-thienyl]-1(methoxymethyl)-4-(trifluoromethyl)- [9CI) (CA INDEX NAME)

MeO-CH2 NH CF3

RN 688325-63-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-(2-propylcyclopropyl)-3-thienyl]-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

He CF3

RN 688325-64-6 CAPLUS
CN 1H-Pytrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-(4-(2-proplycylopropyl)-3-thienyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688323-20-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[2-{1'-methyl{1,1'-bicyclopropyl}-2-y1)-3-thienyl}-4-{trifluoromethyl}- (9CI) (CA INDEX NAME)

Me N CF3

RN 688323-21-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-{2-(1'-methyl[1,1'-bicycloptopyl]-2-yl}-3-thienyl]- (9CI) (CA INDEX NAME)

Me N C-NH S

RN 688323-22-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-[2-(1'-methyl{1,1'-bicyclopropyl}-2-yl)-3-thienyl]- (9CI) (CA INDEX NAME)

RN 688323-23-1 CAPLUS
CN 1H-Fyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-{2-(1'-methyl{1,1'-bicyclopropyl]-2-yl)-3-thienyl}- (9C1) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688325-66-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-[2-(1-methylethyl)cyclopropyl]-3-thienyl]-4-(trifiuoromethyl)- (9CI) (CA INDEX NAME)

Me N CF3

RN 688325-67-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-{difluoromethyl}-1-methyl-N-{4-{2-{1-methyl-thyl}cyclopropyl}-3-thienyl}- (9CI) (CA INDEX NAME)

Me O C-NH S

RN 688325-68-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-[4-[2-(1-methylethyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

CH₂F

RN 688325-69-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[4-{2-(1-methylethyl)-cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688325-70-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1-ethyl-4-methyl-N-[4-[2-(1-methylethyl)cyclopropyl]-3-thienyl)- (9CI) (CA INDEX NAME)

Me O II C-NH-S

RN 688325-71-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-[4-[2-(1-methylethyl)cyclopropyl)-3-thienyl]- [9CI) (CA INDEX NAME)

Me O C NH S

RN 688325-72-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-ethyl-2-fluoro-4-methyl-N-[4-[2-{1-methylethyl)cyclopropyl]-3-thienyl}- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 688325-76-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-(2-butylcyclopropyl)-3-thienyl]-2-fluoro1,4-dimethyl- (9CI) (CA INDEX NAME)

Me C-NH S

RN 688325-77-1 CAPLUS
CN 1H-Fyrrole-3-carboxamide, N-[4-(2-butylcyclopropyl)-3-thienyl]-2-chloro1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688325-78-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-(4-[2-(2-methylpropyl)cyclopropyl)-3thienyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me CF3

RN 688325-79-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[4-[2-(2-methylpropyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

Me N C-NH S
CHF2

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688325-73-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-2-fluoro-1-methyl-N-[4[2-(1-methylethyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

C1-CF2 O | C-NH S

RN 688325-74-8 CAPLUS
CN | H-Pyrrole-3-carboxamide, N-[4-(2-butylcyclopropyl)-3-thienyl]-1-methyl-4(trifluoromethyl)- (9C1) (CA INDEX NAME)

Me N C-NH S

RN 688325-75-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{4-(2-butylcyclopropyl)-3-thienyl}-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

Me O CHF2

LIO ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 688325-80-6 CAPLUS
CN IM-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-[4-{2-(2-methylpropyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

Me O C-NH S

RN 688325-81-7 CAPLUS

(N 1H-Pyrrole-3-carboxamide, 1-(methoxymethyl)-N-[4-[2-(2-methylpropyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

MeO-CH₂ N C-NH S

RN 688325-82-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-(4-[2-[2-methylpropyl)cyclopropyl]-3-thlenyl]- (9C1) (CA INDEX NAME)

Me O O NH S

RN 688325-83-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[4-[2-(2-methylpropyl)gyclopropyl)-3-thlenyll- (9CI) (CA INDEX NAME)

Ne 0 C NH S

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

688325-84-0 CAPLUS
1H-Pyrcole-3-carboxamide, N-[4-[2-(1,1-dimethylethyl)cyclopropyl]-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688325-85-1 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-N-{4-{2-(1,1-dimethylethyl)cyclopropyl}-3-thienyl}-1-methyl- (9CI) (CA INDEX NAME)

688325-86-2 CAPLUS
1H-Pyrole-3-carboxamide, N-[4-[2-(1,1-dimethylethyl)cyclopropyl]-3-thienyl]-2-fluoro-1,4-dimethyl- [9CI) (CA INDEX NAME)

688325-87-3 CAPLUS
1H-Pyrrole-3-carboxamide, 2-chloro-N-[4-[2-(1,1-dimethylethyl)cyclopropyl]-3-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-(4-[2-(3-methyl)butyl)cyclopropyl)-3-thienyl]- (SCI) (CA INDEX NAME)

688325-92-0 CAPLUS
IH-Pyrrole-3-carboxamide, N-(4-(2-hexylcyclopropyl)-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688325-93-1 CAPLUS
1H-Pyrrole-3-carboxamide, N-(4-[1,1'-bicyclopropy1]-2-y1-3-thieny1)-1-methy1-4-(trifluoromethy1)- (9CI) (CA INDEX NAME)

688325-94-2 CAPLUS IN-97rcole-3-carboxamide, N-(4-[1,1'-bicyclopropyl]-2-yl-3-thienyl)-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

688325-95-3 CAPLUS
1H-Pyrrole-3-carboxamide, N-(4-[1,1"-bicyclopropyl]-2-yl-3-thienyl)-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

688325-88-4 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[4-[2-(1,1-dimethylethyl)cyclopropyl]-3-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

688325-89-5 CAPLUS
IH-Pyrrole-3-carboxamide, 1-methyl-N-[4-(2-pentylcyclopropyl)-3-thienyl]-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

688325-90-8 CAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-[2-(3-methylbutyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688325-91-9 CAPLUS

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688325-96-4 CAPLUS 1H-Pyrrole-3-carboxamide, N-(4-{1,1'-bicyclopropyl}-2-yl-3-thienyl)-2-chloro-1,4-dimethyl- (9CI) (CA INDEX NAME)

688325-97-5 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-(2-cyclobutylcyclopropyl)-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) [CA INDEX NAME]

688325-98-6 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-(2-cyclobutylcyclopropyl)-3-thienyl]-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

688325-99-7 CAPLUS IN-[4-(2-cyclopentylcyclopropyl)-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688326-00-3 CAPLUS IN-Pyrrole-3-carboxamide, N-[4-(2-cyclopentylcyclopropyl)-3-thienyl]-4-(difluoromethyl)-1-methyl- (SCI) (CA INDEX NAME)

688326-01-4 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-(2-cyclopentylcyclopropyl)-3-thienyl]-4-(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688326-05-8 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-{2-cyclohexylcyclopropyl)-3-thienyl}-1-methyl-4-(trifluoromethyl)- {9CI} (CA INDEX NAME)

688326-06-9 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-(2-cyclohexylcyclopropyl)-3-thienyl]-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

688326-07-0 CAPLUS
1H-Pytrole-3-carboxamide, N-{4-(2-cyclohexylcyclopropyl)-3-thienyl}-4(fluoromethyl)-1-methyl- {9CI} (CA INDEX NAME)

Page 2030/08/2005

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688326-02-5 CAPLUS
1H-Pytrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[4-{2-cyclopentylcyclopropyl}-3-thienyl}-1-methyl- (9CI) (CA INDEX NAME)

688326-03-6 CAPLUS
IH-Pyrrole-3-carboxamide, N-[4-(2-cyclopentylcyclopropyl)-3-thienyl]-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

688326-04-7 CAPLUS 1H-Pyrrole-3-carboxamide, 2-chloro-N-[4-(2-cyclopentylcyclopropyl)-3-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 688326-08-1 CAPLUS
CN | H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[4-(2cyclohexylcyclopropyl)-3-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

688326-09-2 CAPLUS
1H-Pyrrole-3-carboxamide, N-{4-(3-cyclohexyl-2,2-difluorocyclopropyl)-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688326-10-5 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-(2-cyclohexylcyclopropyl)-3-thienyl]-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

688326-11-6 CAPLUS
1H-Pyrcole-3-carboxamide, 2-chloro-N-[4-(2-cyclohexylcyclopropyl)-3-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

688326-12-7 CAPLUS

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN H-Pyrrole-3-carboxamide, N-[4-(2-cycloheptylcyclopropyl)-3-thienyl]-1methyl-4-(trifluoromethyl)-(5C1) (CA INDEX NAME)

688326-13-8 CAPLUS
1H-Pytrole-3-carboxamide, N-(4-(2-cycloheptylcyclopropyl)-3-thienyl]-1-ethyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

698326-15-0 CAPLUS
1H-Pyrrole-3-carboxamide, N-{4-(2-cycloheptylcyclopropyl)-3-thienyl}-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

688326-16-1 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-(2-cycloheptylcyclopropyl)-3-thienyl]-4(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

688326-21-8 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-(2-cyclooctylcyclopropyl)-3-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

688326-22-9 CAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-(2-phenylcyclopropyl)-3-thienyl]-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

688326-23-0 CAPLUS 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[4-{2-phenylcyclopropyl)-3-thienyl}- (9CI) (CA INDEX NAME)

688326-24-1 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-(4-(2-phenylcyclopropyl)-3-thienyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688326-17-2 CAPLUS 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-{4-(2-cycloheptylcyclopropyl)-3-thienyl)-2-fluoro-1-methyl- (9CI) (CA INDEX NAME)

688326-18-3 CAPLUS IM-Pyrrole-3-carboxamide, N-[4-(2-cycloheptylcyclopropyl)-3-thienyl]-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

688326-19-4 CAPLUS 1H-Pyrrole-3-carboxamide, 2-chloro-N-[4-(2-cycloheptylcyclopropyl)-3-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

688326-20-7 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-(2-cyclooctylcyclopropyl)-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9Cl) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688326-25-2 CAPLUS
1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-[4-(2-phenylcyclopropyl)-3-thienyl]- {9CI} (CA INDEX NAME)

688326-26-3 CAPLUS
1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-{4-(2-phenylcyclopropyl)-3-thienyl]- (SCI) (CA INDEX NAME)

688326-27-4 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-(2-(4-fluorophenyl)cyclopropyl]-3-thienyl]-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688326-28-5 CAPLUS
1H-Pytrole-3-carboxamide, 4-(difluoromethyl)-N-[4-[2-(4-fluorophenyl)cyclopropyl]-3-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688326-29-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-[2-(4-chlorophenyl)cyclopropyl]-3-thienyl]l-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688326-30-9 CAPLUS
CN 1H-Fyzrola-3-carboxamide, N-[4-[2-(4-chloropheny1)cyclopropy1]-3-thieny1]4-(difluoromethy1)-1-methy1- (9C1) (CA INDEX NAME)

RN 688326-31-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-[2-[4-bromophenyl]cyclopropyl]-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688326-32-1 CAPLUS CN 1H-Pyrrole-3-carboxamide, N-[4-[2-(4-bromophenyl)cyclopropyl]-3-thienyl]-4-

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688326-36-5 CAPLUS
CN 1H-Pyrcole-3-carboxamide, N-{4-[2-(3-furanyl)cyclopropyl}-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688326-37-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-{4-(1'-methyl{1,1'-bicyclopropyl}-2-yl)-3-thienyl}-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688326-38-7 CAPLUS
CN lH-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[4-(1'-methyl[1,1'-bicyclopropyl]-2-yl)-3-thienyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) (difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688326-33-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-[2-(2-thienyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688326-34-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-[2-(3-thienyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688326-35-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{4-{2-(2-furanyl)cyclopropyl}-3-thienyl}-1-methyl-4-(trifluoromethyl)- {9CI} (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continue

RN 688326-39-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-(4-(1'-methyl[1,1'-bicyclopropyl]-2-yl)-3-thienyl]- (9CI) (CA INDEX NAME)

RN 688326-40-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-(4-(1'-methyl[1,1'-bicyclopropyl]-2-yl)-3-thienyl]- (9CI) (CA INDEX NAME)

RN 688328-21-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-{(1R,2R)-2-(1,1-dimethylethyl)cyclopropyl}-3-thienyl}-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688328-22-5 CAPLUS
HH-Pyrrole-3-carboxamide, N-[2-(1R,25)-[1,1'-bicyclopropyl]-2-yl-3-thienyl]-1-methyl-4-(trifluoromethyl)-, rel- (901) (CA INDEX NAME)

Relative stereochemistry.

688328-23-6 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-[(1R.ZR)-2-(4-fluorophenyl)cyclopropyl]-3-thienyl]-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 14 Apr 2004

AB DNA binding ligands with potent antimicrobial activity against Gram-pos.
bacteria were further optimized by variation of the internal aromatic amino
acids. This modification led to compds. with improved in vivo efficacy in
lethal murine models of peritonitis (methicillin-resistant 5. aureus,
MRSA) and lung infection (5. pneumoniae).

ACCESSION NUMBER: 2004:30252 CAPLUS

DOCUMENT NUMBER: 2004:30252 CAPLUS

DOCUMENT NUMBER: 141:64377

DNA binding ligands with in vivo efficacy in murine
models of bacterial infection: optimization of
internal aromatic amino acids

Burli, Roland W.; Kaizeman, Jacob A.; Duan, Jian-Xin;
Jones, Peter: Johnson, Kirk W.; Iwamoto, Mari: Truong,
Klet: Hu, Wenhao: Stanton, Timothy; Chen, Alfred:
Touami, Sofia: Gross, Matthew; Jiang, Vernon: Ge,
Yigong; Moser, Heinz E.
Genesoft Pharmaceuticals, South San Francisco, CA,
94080, USA

Bioorganic & Medicinal Chemistry Letters (2004),
14(9), 2067-2072
CODEN: EMCLES: ISSN: 0960-894X

Elsevier Science B.V.

DOCUMENT TYPE: Journal
LANGUAGE: English

DOCUMENT TYPE: LANGUAGE: IT 710950-17-7 Journal English

710950-17-7

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(DNA binding ligands with in vivo efficacy in murine models of bacterial infection and structure-activity relationship)
710950-17-7 CAPLUS
3-Isoquinolinecarboxamide, N-[1-methyl-5-[[[5-[[[1-methyl-5-[[[2-(4-morpholiny)] ethyl]amino]carbonyl]-1H-pyrrol-3-yl]amino]carbonyl]-3-thienyl]amino]carbonyl]-1H-pyrrol-3-yl]- (SCI) (CA INDEX NAME)

PAGE 1-B

REFERENCE COUNT:

THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688328-24-7 CAPLUS cosize-z4-/ CAPLUS
IH-Pyrrole-3-carboxamide, N-{2-{(1R,2R)-2-{4-chlorophenyl)cyclopropyl}-3thienyl}-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 21 Dec 2003

AB The invention relates to synthetic excitatory amino acid prodrugs for the treatment of neurol. disorders and psychiatric disorders. Bicyclic amino acids I (A is H-Q1-10, where Q is aminoacyl; X is O, S, SO, SO2, or substituted methylener, RI is H or F: R2 is H, F, or ORI) or their pharmaceutically-acceptable salts are claimed. Thus, prodrug II.HCl was prepared via peptide coupling reaction and shown to exhibit comparable concentration in rat plasma to that of the non-prodrug form.

ACCESSION NUMBER:

100:42463

101:42463

101:42463

101:42463

101:42463

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102:42463

103:42463

104:42463

104:42463

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109:4246

PR

FAMILY ACC. NUM. COUNT:

PAT	ENT	NO.			KIN	D	DATE		- 2	APPL	ICAT:	ION	NO.		D.	ATE	
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WO	2003	1042	17		A2		2003	1218	1	WO 2	003-1	JS15	405		2	0030	606
WO	2003	1042	17		A3		2004	0226									
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GΕ,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	15,	JP,	KE,	KG,	K₽,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA.	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
		PH,	PL,	PT,	RO,	RU,	sc,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,
		TZ,	UΑ,	UG,	US,	UZ,	ν¢,	٧N,	YU,	ZA,	ZM,	ZW					
	RW:	GH,	GΜ,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
		KG,	ΚZ,	MD,	RU,	ŦJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	ΚU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
		BF,	BJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TĐ,	ŤG
CA	2488	167			AA		2003	1218		CA 2	003-	2488	167		2	0030	606
EP	1517	915			A2		2005	0330		EP 2	003-	7572	66		2	0030	606
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SÈ,	MC,	PT,
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK	
ORITY	APP	LN.	INFO	. :						EP 2	002-	3801	20		A 2	0020	611
										EP 2	002-	3801	21		A 2	0020	611
										US 2	002-	4159	36P		P 2	0021	003

L10 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN US 2002-415937P (Continued) P 20021003 W 20030606 WO 2003-US15405 MARPAT 140:42463

635317-69-07
RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of prodrugs of excitatory amino acids)
635317-69-0 CAPLUS
2-Thiabicyclo[3.1.0]hexane-4,6-dicarboxylic acid, 4-[[(2S)-1-[(1,1-dimethylethoxylcarbonyl]-2-pyrrolidinyl]carbonyl]amino]-, dimethyl ester,
2,2-dioxide, (1R,4S,5S,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L10 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

JP 2005502703 T2 20050127 JP 2003-256882 20020909

US 2005014700 A1 20050120 US 2004-489006 20040827

PRIORITY APPLN. INFO.: W 2002-181179P P 20010909 OTHER SOURCE(S): MARPAT 138:255007

IT 372953-56-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Uses)
(aynthesis and evaluation of tetrahydrocyclopropa[c]benz[e]indol-4-one analogs of CC-1065 and the duocarmycins defining the contribution of the DNA-binding domain)
372953-56-5 CAPLUS
Carbamic acid, [5-[[[5-[[[3]]-1-(chloromethyl)-1,2-dihydro-5-hydroxy-3H-benz[e]indol-3-yl]carbonyl]-3-thienyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

502171-77-9P

502171-77-99
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and evaluation of tetrahydrocyclopropa[c]benz[e]indol-4-one analogs of CC-1065 and the duocarmycins defining the contribution of the DNA-binding domain)
502171-77-9 CAPLUS
2-Thiophenecarboxylic acid, 4-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

ANSWER 6 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 21 Mar 2003

AB 132 CBI analogs I [X, Y = arylene, heteroarylene] of CC 1065 and the duocarmycins having dimeric monocyclic, bicyclic, and tricyclic heteroaroms. substituents were synthesized by a parallel route. The resultant analogs were evaluated with respect to their catalytic and cytotoxic activities. The relative contribution of the various dimeric monocyclic, bicyclic, and tricyclic heteroaroms, substituents within the DNA binding domain were characterized. Several of the resultant CBI analogs of CC 1065 and the duocarmycins were characterized as having enhanced catalytic and cytotoxic activities and were identified as having utility as anti-cancer agents. Thus, I (X = Y = -4-C6H4-) was prepared starting from 4-H2NNG6H4CO2H and the hydrochloride salt of seco-CBI.

ACCESSION NUMBER: 2003:221652 CAPLUS
DOCUMENT NUMBER: 138:255007

TITLE: Preparation of CBI analogues of CC 1065 and the duocarmycins for therapeutic use as anticancer agents Boger, bale L.

PATENT ASSIGNEE(S): The Scripps Research Institute, USA
CODEN: PIXAD2
PATENT TYPE: Patent
LANGUAGE: English

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA	TENT	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D.	ATE	
						-									_		
WO	2003	0228	06		A2		2003	0320	1	WO 2	002-	US28	749		2	0020	909
WO	2003	0228	06		A3		2003	1113									
	W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT.	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX.	MZ,	NO,	NZ,	OM,	PH,
		PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	TZ,
		UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZM,	ZW							
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	52,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
		KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	SK,	TR,	BF,	ВJ,	CF,
		CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG			
CA	2459	308			AA		2003	0320		CA 2	002-	2459	308		2	0020	909
EP	1423	110			A2		2004	0602		EP 2	002-	7982	01		2	0020	909
	D -	TA.	BE.	CH.	DE.	DK.	ES.	FR.	GB.	GR.	TT.	1.1	1.11	NT.	SE.	MC.	PT.

ANSWER 7 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 02 Jan 2003

AB Title compds. I (wherein R1 and R6 = independently H, halo, CF3, alkyl, alkylthio, alkoxy, CN, NO2, NH2, Ph, OPh, SPh, CH2Ph, OCH2Ph, SCH2Ph, or (un) substituted amido, carbamido, sulfonyl, etc.: R2 = H, halo, CF3, OH, alkyl, alkoxy, CHO, CN, NO2, (un) substituted amino, or alkylaulfonyl: R3 = CO2H, OPO3H2, SO3H, etc.: R4 = H, CF3, alkyl, alkoxy, (alkyl)cycloalkyl, CHO, halo, etc.: R5 = alkyl, alkoxy, (alkyl)cycloalkyl, etc.: and pharmaceutically acceptable salts thereof) were prepared as phospholipase enzyme inhibitors. For example, 5-nitrondole was c3-alkylated (55%) with M6 4-(bromomethyl)-3-methoxybenzoate in dioxane, N-alkylated (57%) with 1-iodopropane in a solution of THF and NaH, and converted to the amine (80%) by hydrogenation using Pt/C. The amine was converted to the carbamate (39%) by addition of cyclopentyl chloroformate in CH2Cl2 and 4-methylmorpholine, and the resultant ester was hydrolyzed to yield II (71%). The latter inhibited cytosolic phospholipase A2 (CPLAZ) by 50% at a concentration of 170 M in a coumarin assay and reduced footpad volume by 16.61% at a dose of 5 mg/Kg IV in a carrageenan-induced footpad edema test on rats. Thus, I are useful for treatment of infilammatory conditions, such as arthritis, inflammatory bowel disease, and asthma (no data).

ACCESSION NUMBER: 2003:1275 CAPLUS

DOCUMENT NUMBER: 138:55866 TITLE:

Preparation of indole derivatives as phospholipase enzyme inhibitors for treatment of inflammatory conditions conditions Seehra, Jasbir S.; McKew, John C.; Lovering, Frank; Bemis, Jean E.; Xiang, Yibin: Chen, Lihren: Knopf, INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

John L. Genetics Institute, LLC, USA U.S., 57 pp., Cont.-in-part of U.S. Ser. No. 256,062, abandoned.

CODEN: USXXAM English

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT:

PATENT NO. KIND DATE APPLICATION NO. DATE US 2000-686616 US 1998-113674P US 1999-256062 US 6500853 PRIORITY APPLN. INFO.: 20001011 20021231 Bl

OTHER SOURCE(S): MARPAT 138:55866

IT 241497-74-5DP, 3-Thiophenecarboxylic acid, 4-[[5[(cyclopentylcarbonyl)amino]-1-(diphenylmethyl)-1H-indol-3yl]carbonyl]amino]-, ester
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT

RL: RCT (Reactant); SPN (Synthetic preparation); rncr (resparation); one (Reactant or reagent) (intermediate; preparation of indole derivs, as phospholipase enzyme inhibitors for treatment of inflammatory conditions) 241497-74-5 CAPLUS 3-Thiophenecarboxylic acid, 4-[{[5-((cyclopentylcarbonyl)amino}-1-(diphenylmethyl)-1H-indol-3-yl]carbonyl]amino}- (9CI) (CA INDEX NAME)

241497-74-5P, 3-Thiophenecarboxylic acid, 4-{{(5-(cyclopentylcarbonyl)amino)-1-(diphenylmethyl)-1H-indol-3-yl]carbonyllamino}-RE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Uses)
 (phospholipase inhibitor: preparation of indole derivs. as phospholipase
 enzyme inhibitors for treatment of inflammatory conditions)
241497-74-5 CAPLUS
3-Thiophenecarboxylic acid, 4-[[[5-[(cyclopentylcarbonyl)amino]-1(diphenylmethyl)-1H-indol-3-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 20 Dec 2002

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Title compds. I [R1 = H, F, C1, CN, CF3, OH, N(R2)2, OR2, etc.; R2-3 = H, alkyl, heteroalkyl; n = 1-25; Y = alkylene, (hetero)aromatic; Z = O, N; m = 1 if Z = O, m = 2 if Z = N] were prepared For instance, II (preparation given)

coupled to 4-chloro-2-fluorobenzoic acid, the product saponified and the resulting carboxylic acid coupled to N-(2-aminoethyl)morpholine to give III. III had MIC \$4 ug/mL against B. cereus, E. faecalis, E. faecium, S. aureus, S. epidermidis and S. pneumoniae. A number of compds. of the invention were screened for their ability to bind to three DNA sites (binding data tabulated).

ACCESSION NUMBER: 2002:964476 CAPLUS
DOCUMENT NUMBER: 138:39101

TITLE: Preparation of antipathogenic poly-pyrrole-benzamide compounds
INVENTOR(S): Burli, Roland W.; Kaizerman, Jacob A.; Jones, Peter PATENT ASSIGNEE(S): Genesoft, Inc., USA
SOURCE: PIXXDZ

COODE: PIXXDZ

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	WO 20	02				A3		2003											
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			LS,	LT,	LU,	LV,	MA,	MD,	MG,	ΜK,	MN,	MW,	ΜX,	ΜZ,	NO,	NZ,	OM,	PH,	
			PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	
			UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZM,	ZW								
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			GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG								
	US 20	032	2361	98		A1		2003	1225		US 2	002-	1657	64		2	0020	606	
PRIOR	RITY A	PPI	LN.	INFO	. :						US 2	001-	2982	06P		P 2	0010	613	
											US 2	001-	3423	09P		P 2	0011	221	
OTHER	SOUR	CE	(S):			MAR	PAT	138:	3910	1									
IT	47880	3-5	8-61	>															
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	morph	01:	inyl) eth	y1]a:	mino	Car	bony	1]-3	-thi	enyl	1- (9CI)	{C	A IN	DEX	NAME)	
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L10 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L10 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

L10 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 09 Aug 2002

AB Title compds. [I; X = (substituted) (CH2)m; m = 1-3; R1 = (substituted) alkyl, alkenyl, alkynyl, aryl, heteroaryl, etc.; R2, R3 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R4, R41, R5, R51 = H, OH, (substituted) alkyl, alkynyl, cycloalkyl, aryl, heteroaryl, alkoxy, etc.; R6, R61 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aryl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R7, R8 = (substituted) (CH2)HH; n = 1-4; R7RBN = (substituted) alkyl, alkenyl, aryl, heteroaryl, etc.; R7, R8 = (substituted) (CH2)HH; n = 1-4; R7RBN = (substituted) cycloheteroalkyl), were prepared as cardiovascular agents (no data). 974 I, including (II), were prepared accession NUMBER: 2002:594840 CAPLUS
DOCUMENT NUMBER: 2002:594840 CAPLUS

TITLE:

137:154858
Preparation of arylsulfonamidopiperidones as inhibitors of Factor Xa.
Stein, Philip P.; O'Connor, Stephen P.; Lawrence, R. Michael: Shi, Yan
Bristol-Myers Squibb Company, USA
PCT Int. Appl., 246 pp.
CODEN: PIXXD2
Patent INVENTOR(S):

PATENT ASSIGNEE(S):

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PATENT NO.						DATE			APPL						ATE	
															-		
WO	2002	0608	94		A2		2002	0808	,	WO 2	002-	US 25	42		2	0020	128
WO	2002	0608	94		A3		2002	1219									
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		co,	CR,	CU,	CZ.	DE,	DK.	DM.	DZ.	EC.	EE,	ES,	FI.	GB,	GD,	GE.	GH,
		GM,	HR,	HU,	ID.	IL.	IN,	IS.	JP.	KE.	KG.	KP,	KR.	KZ,	LC.	LK.	LR,
		LS.	LT.	LU.	LV.	MA.	MD.	MG.	MK.	MN.	MW.	MX.	MZ.	NO.	NZ.	OM.	PH.
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EP	1358	178			A2		2003	1105		EP 2	002-	7173	B 1		2	0020	128
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	LT.	LV,	FI,	RO,	MK,	CY,	AL,	TR						
JF	2004	5186	88		T2		2004	0624		JP 2	002-	5610	43		2	0020	128
US	6555	542			B1		2003	0429		US 21	002-	5962	1		2	0020	129
PRIORIT	APP	LN.	INFO.	. :						US 2	001-	2649	54P		P 2	0010	130

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 18 May 2002

AB The title compds. [1: X = 0, 5: Rl = CF3, CF2H, CFH2; R2 = alkyl, haloalkyl, alkoxyalkyl, haloalkoxyalkyl; R3 = H, Me, CF3, F; Q = substituted Ph, 2-thienyl, 3-thienyl which have plant-protecting properties and are suitable for protecting plants against infestation by phytopathogenic microorganisms, were prepared Thus, treating l-methyl-4-trifluoromethylpyrrole-3-carboxylic acid with oxalyl chloride in the presence of a catalytic amount of DMF in CH2Cl2 followed by addition of the resulting acid chloride to a solution of 2-(1,3-dimethylbutyl)phenylamine and Et3N in CH2Cl2 afforded II. Compds. I showed good activity (< 20% infestation) against Puccinia recondita (brown rust) on wheat.

ACCESSION NUMBER: 2002:368451 CAPLUS
DCCUMENT NUMBER: 136:369602

TITLE: Preparation of pyrrolecarboxamides and pyrrolecarbotiosmides as agrochemical fungicides

136:369602
Preparation of pyrrolecarboxamides and pyrrolecarbothioanides as agrochemical fungicides Walter, Harald Syngenta Participations A.-G., Switz. PCT Int. Appl., 66 pp. CODEN: PIXXD2
Patent

INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

LANGUAGE: E FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PAT							DATE				LICAT				D.	ATE	
						-									-		
WO	2002	0385	42		A1		2002	0516		WO :	2001-	EP12	830		2	0011	106
	W:	ΑE,	AG,	AL,	AM,	AT,	ΑU,	ΑZ,	BA,	BB	, BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC	, EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GΜ,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE	, KG,	KP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG.	MK,	MN	, MW,	MX,	MZ,	NO,	NZ,	PH,	PL,
		PT,	RO,	RU,	SD,	SE,	5G,	SI,	5K,	SL	, TJ,	TM,	TR,	TT,	TZ,	UA,	UG,
		US,	UZ,	VN,	YU,	ZA,	ZW,	AM,	AZ,	BY	, KG,	KZ,	MD,	RU,	TJ,	TM	
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ	, TZ,	UG,	ZW,	AT,	BE,	CH,	CY
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		BJ,	CF.	CG.	CI.	CM,	GΑ,	GN,	GQ,	G₩	, ML.	MR.	NE,	SN,	TD,	TG	
CA	2426	033			AA		2002	0516		CA :	2001-	2426	033		2	0011	106
ΑU	2002	0236	68		A5		2002	0521		AU .	2002-	2366	8		2	0011	106
ΕP	1341	757			A1		2003	0910		EP.	2001-	9935	99		2	0011	106
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		IE.	SI.	LT.	LV.	FI.	RO,	MK,	CY,	AL	. TR						
BR	2001	0152	00		A		2004	0217		BR .	2001-	1520	0		2	0011	106
EG	2312	2			А		2004	0428		ĒG .	2001-	1173			2	0011	106
JΡ	2004	5131	63		T2		2004	0430		JP .	2001- 2002-	5410	78		2	0011	106
US	2005	1191	30		Al		2005	0602		us	2003-	4162	10		2	0011	

Page 2630/08/2005

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L10 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) Wo 2002-US2542 W 20020128
OTHER SOURCE(S): MARPAT 137:154858
IT 445277-00-99
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use): BIOL (Biological study); PREP (Preparation); USES
          (preparation of arylsulfonamidopiperidones as inhibitors of Factor Xa) 445277-00-9 CAPLUS
         2-Pyrolidinecarboxamide, 1-[[(3S)-3-[[[(1E)-2-(5-chloro-2-thieny)]ethenyl]sulfonyl]amino|-2-oxo-1-piperidinyl]acetyl]-N-(tetrahydro-1,1-dioxido-3-thienyl)-, (2S)- (9CI) (CA INDEX NAME)
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Absolute stereochemistry. Double bond geometry as shown.

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L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS ON STN ZA 2003003012 A 20040520 ZA 2003-3012 GB 2000-27284 GB 2000-30268
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A 20001108
A 20001212
W 20011177
OTHER SOURCE(S): MARPAT 136:369602

IT 424932-40-6P 424932-41-7P 424932-42-8P
424932-43-9P 424932-44-0P 424932-45-1P
424932-46-2P 424932-45-1P
424932-46-5P 424932-55-6P 424932-45-1P
424932-55-5P 424932-55-5P 424932-51-5P
424932-53-3P 424932-55-6-4P 424932-57-5P
424932-58-6P 424932-55-6-4P 424932-63-3P
424932-61-1P 424932-62-2P 424932-63-3P
424932-64-4P 424932-65-6P
424932-67-7P 424932-68-6P
424932-73-5P 424932-73-7P
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4
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                                                                                      RL: AGR (Agricultural use): BSU (Biological study, unclassified): SPN (Synthetic preparation): BIOL (Biological study): PREP (Preparation): USES
                                                                                  (Usea) (preparation of pyrrolecarboxamides and pyrrolecarbothioamides as agrochem. fungicides) 42432-40-6 CAPLUS (1432-40-6 CAPLUS (1432-4
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424832-41-7 CAPLUS 1H-Pyrrole-3-carboxamide, N-[2-(1,3-dimethylbutyl)-3-thienyl]-1-(methoxymethyl)-4-(trifluoromethyl)- (9C1) (CA INDEX NAME)

424832-42-8 CAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[2-(3-methyl-1-(trifluoromethyl)butyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CF3 1-Bu-CH 0 1-Bu-CH 0 1-NH-CH NH-Me

RN 424832-43-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-4-(trifluoromethyl)-N-[2-[4,4,4-trifluoro-1-methyl-3-(trifluoromethyl)butyl)-3-thienyl]- (9CI) (CA INDEX NAME)

RN 424832-44-0 CAPLUS
CN HH-Pytrole-3-carboxamide, N-[2-(1,3-dimethylpentyl)-3-thienyl)-1-methyl-4(trifluoromethyl)- (SCI) (CA INDEX NAME)

Me Me Et-CH-CH2-CH NH-C

RN 424832-45-1 CAPLUS
CN 1H-Fyrrole-3-carboxamide, N-[2-(1,3-dimethylpentyl)-3-thienyl]-1(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 424832-49-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1,3-dimethylbutyl)-3-thienyl]-2-fluoro-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

i-Bu-CH CF3

RN 424832-50-8 CAPLUS
CN 1H-Pyrcle-3-carboxamide, N-[2-(1,3-dimethylbutyl)-3-thienyl}-2-fluoro-1(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 424832-51-9 CAPLUS
CN IN-Pyrrole-3-carboxamide, N-[2-(1,3-dimethylpentyl)-3-thienyl]-2-fluoro-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me Ne Ne CF3

RN 424832-52-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1-methyl-N-[2-{3-methyl-1-

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me | He | CH2 - CH2 - CH4 - CH2 - CH4 - CH2 - CH4 - CH

RN 424832-46-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1,3-dimethylbutyl)-5-fluoro-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me | CH-Bu-i

RN 424832-47-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-[1,3-dimethylbutyl)-4-fluoro-3-thienyl]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me | CH-Bu-1

RN 424832-48-4 CAPLUS
CN lH-Pyrrole-3-carboxamide, N-[2-(3-ethyl-1-methylpentyl)-3-thienyl]-1methyl-4-(trifluoromethyl)- (9C1) (CA INDEX NAME)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) (trifluoromethyl)butyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

CF3 1-Bu-CH O CF3

RN 424832-53-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1-methyl-N-[2-[3-methyl-1-(trifluoromethyl)pentyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me | CF3 | C

RN 424832-54-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-N-[2-(1,3-dimethylbutyl)-3-thienyl]-1-methyl- (9C1) (CA INDEX NAME)

1-Bu-CH | NH-C | N Me

RN 424832-55-3 CAPLUS
CN IH-Pyrrole-3-carboxamide, 4-(difluoromethyl)-N-[2-(1,3-dimethylpentyl)-3-thienyl)-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

424832-56-4 CAPLUS 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[2-[3-methyl-1-(trifluoromethyl)butyl]-3-thienyl]- (9CI) (CA INDEX NAME)

424832-57-5 CAPLUS
1H-Pyrrole-3-carboxamide, N-(2-(1,3-dimethylbutyl)-3-thienyl]-4(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

424832-58-6 CAPLUS 1H-Pyrrole-3-carboxamide, N-{2-(1,3-dimethylpentyl)-3-thienyl}-4-(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

424832-62-2 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(1R,2S,4R)-bicyclo[2.2.1]hept-5-en-2-yl-3-thienyl]-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

424832-63-3 CAPLUS
1H-Pyrrole-3-carboxamide, N-{2-{1R,2R,4\$}-bicyclo{2.2.1}hept-2-yl-3-thienyl}-1-methyl-4-(trifluoromethyl)-, rel- {9CI} (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

424832-59-7 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-{2-{3-methyl-1-{trifluoromethyl}butyl}-3-thienyl}- (9CI) (CA INDEX NAME)

424832-60-0 CAPLUS IN-Pyrole-3-carboxamide, N-(2-bicyclo[2.2.1]hepta-2,5-dien-2-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

424832-61-1 CAPLUS 1H-Pyrrole-3-carboxamide, N-{2-bicyclo{2.2.1}hept-2-en-2-yl-3-thienyl}-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 424832-64-4 CAPLUS
CN | H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4S)-bicyclo[2.2.1]hept-2-yl-4-fluoro3-thienyl]-1-methyl-4-trifluoromethyl-, rel- (9CI) (CA INDEX NAME)

424832-65-5 CAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-4-(trifluoromethyl)-N-[2-[(1R,2S,45)-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl]-3-thienyl]-, rel- [9CI] (CA INDEX NAME)

Relative stereochemistry.

424832-66-6 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(1R, 2R, 4S)-bicyclo{2.2.1}hept-2-yl-3-thienyl}-1-(methoxymethyl)-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

424832-67-7 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4s)-bicyclo[2.2.1]hept-2-yl-3-thienyl]-4-(difluoromethyl)-1-methyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

424832-68-8 CAPLUS 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]octa-2,5-dien-2-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

424832-71-3 CAPLUS
1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

424832-72-4 CAPLUS IH-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-y1-3-thienyl)-1-(methoxymethyl)-4-(trifluoromethyl)- (9Cl) (CA INDEX NAME)

424832-73-5 CAPLUS
1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-4-fluoro-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Page 2930/08/2005

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

424832-69-9 CAPLUS
1H-Pyrrole-3-carboxamide, N-{2-bicyclo[2.2.2]oct-2-en-2-yl-3-thienyl}-1-methyl-4-{trifluoromethyl}- (9CI) (CA INDEX NAME)

424832-70-2 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(1R,2S,4R)-bicyclo[2.2.2]oct-5-en-2-yl-3-thienyl]-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 424832-74-6 CAPLUS
CN | H-Fyrrole-3-carboxamide, N-{2-bicyclo[2.2.2]oct-2-yl-4-fluoro-3-thienyl)|-{methoxymethyl}-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

424832-75-7 CAPLUS 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

424832-76-8 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(1R,2S,4R)-bicyclo[2.2.1]hept-5-en-2-yl-3-thienyl]-2-fluoro-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me N P HN

RN 424832-77-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4S)-bicyclo[2.2.1]hept-2-yl-3-thienyl]-2-fluoro-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry

RN 424832-78-0 CAPLUS

(N 1H-Pyrrole-3-carboxamide, N-{2-(1R,2S,4R}-bicyclo{2.2.1}hept-5-en-2-yl-3-thiepyl]-2-fluoro-1-(methoxymethyl)-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 424832-81-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo{2.2.2}oct-2-yl-3-thienyl)-2-fluoro1-methyl-4-(trifluoromethyl)- (SCI) (CA INDEX NAME)

RN 424832-82-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-2-fluorol-(methoxymethyl)-4-{trifluoromethyl}- (9CI) {CA INDEX NAME}

RN 424832-83-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4S)-bicyclo[2.2.1]hept-2-yl-3-thienyl}-1,2-dimethyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Page 3030/08/2005

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 424832-79-1 CAPLUS
CN HH-Pyrrole-3-carboxamide, N-[2-{IR,2R,4S}-bicyclo[2.2.1]hept-2-yl-3-thienyl]-2-fluoro-1-(methoxymethyl)-4-{trifluoromethyl}-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 424832-80-4 CAPLUS
CN HH-Pyrrole-3-carboxamide, N-[2-(1R,2S,4R)-bicyclo[2.2.2]oct-5-en-2-yl-3-thienyl]-2-fluoro-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued Relative stereochemistry.

RN 424832-84-8 CAPLUS
CN 1H-Pytrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-1,2-dimethyl-4-trifluoromethyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 11 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 21 Dec 2001

AB The development of a solution-phase synthesis of distamycin A and its extension to the preparation of 2640 analogs are described. Thus, solution-phase synthesis techniques with reaction workup and purification employing acid/base siquid-liquid extns. were used in the multistep preparation of distamycin A (8 steps, 40 overall yield) and a prototypical library of 2640 analogs providing intermediates and final products that are 2 95 pure on conventional reaction scales. Screening the prototypical library provided compds. that are 1000 times more potent than distamycin A in cytotoxic assays (I, Boc = tert-butoxycarbonyl, IC50 = 29 nM, Ll210), that bind to poly(dA]-poly(dT) with comparable affinity, and that exhibit an altered DNA binding sequence selectivity. Several candidates were identified which bound the five base-pair AT-rich site of the PSA-ARE-3 sequence, and one (II, R = 4-dimethylaminobutyryl; K = 3.2 x 106 M-1) maintained the high affinity binding (K = 4.5 x 106 M-1) to the ARE-consensus sequence containing a GC base-pair interrupted five base-pair AT-rich site suitable for inhibition of gene transcription initiated by hormone insensitive androgen receptor dimerization and DNA binding characteristic of therapeutic resistant processors.

ACCESSION NUMBER: 2001-923774 CAPLUS

2001:923774 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 136:54024

Preparation of distamycin A analogs and screening for DNA binding and cytotoxic activities TITLE:

L10 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 11 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) Boger, Dale L. Scripps Research Institute, USA PCT Int. Appl., 93 pp. CODEN: PIXXD2 PATENT ASSIGNEE (S): DOCUMENT TYPE: LANGUAGE: Patent English 2 FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE WO 2001096313 20011220 WO 2001-US19404 20010614 W0 2001095313 A1 20011220 W0 2001-US19404 20010614
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MX, MN, MM, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: CH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, SE, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO:: US 2000-211760P P 20000614

TT 292069-27-3P 292069-37-5P

RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); TMI A1

292069-27-39 292069-37-5P

RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU
(Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study);

PREP (Preparation); USES (Uses)
(preparation of distamycin A analogs and screening for DNA binding and
cytotoxic activities)
292069-27-3 CAPLUS
Benzo(1, 2-b:4, 3-b')dipyrrole-2-carboxylic acid, 6-[[4-[[[4-[(1,1dimethylethoxylcarbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-2thienyl]carbonyl]-3,6,7,8-tetrahydro-, methyl ester (9CI) (CA INDEX NAME)

292069-37-5 CAPLUS

Benzo(1,2-b:4,3-b'|dipyrrole-2-carboxylic acid, 6-[[4-[[4-[4-(dimethylamino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-2-thienyl]carbonyl]-3,6,7,8-tetrahydro-, methyl ester (9CI) (CA INDEX NAMP)

L10 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 12 Oct 2001

AB Charged compds. are provided that have one or more regions of localized pos. charge, as are compns. comprising such compds., methods of synthesizing such compds. to identify those having anti-infective activity, and methods of using such compds. to prevent or inhibit infections. These compds., and compns. containing them, have multiple applications, including use in human and animal medicine and in agriculture.

ACCESSION NOMER: 201:747848 CAPLUS

DOCUMENT NUMBER:

2001:747848 CAPLUS
133::298753
Charged compounds having a nucleic acid-binding molety, their preparation, and their use as antiinfective agents
Ge, Yigong, Taylor, Matthew J.; Baird, Eldon E.;
Moser, Heinz E.; Burli, Roland W.
Genesoft, Inc. USA
PCT Int. Appl., 62 pp.
CODEN: PIXXD2
Patent

INVENTOR (S):

PATENT ASSIGNEE(S):

SOURCE:

English

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

											LICAT						
						-											
										WO	2001-	US82:	52		- 2	20010	314
WO	2001	7489	98		A3		2003	0116									
	W:	AE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB	, BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		CR,	CU,	CZ,	DΕ,	DK,	DM,	DZ,	EE,	ES	, FI,	GB,	GD,	GΕ,	GH,	GM,	HR,
		HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP	, KR,	KZ,	LC,	LK,	LR,	LS,	LT,
		LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX	, MZ,	NO,	NZ,	PL,	PT.	RO,	RU,
											, TT,						
											, TJ,						
	RW:										, TZ,		ZW.	AT.	BE.	CH.	CY.
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CA	2403										2001-						314
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110	2002										2002-	2788	70			20021	022
PRIORITY																	
FKIOKIII	AFF		11110								2001-						
											2001-						

OTHER SOURCE(S): MARPAT 135:298753

365211-00-3 RE: BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): THU (Therapeutic use): BIOL (Biological study); USES (Uses)

(charged compds. with nucleic acid-binding moiety, preparation, and use as

(charged compds. with nucleic acid-binding moiety, preparation, and use antiinfective agents)
365211-00-3 CAPLUS
3-Isothiazolecarboxamide, 4-chloro-5-[[3-(dimethylamino)propyl]amino]-N-[5-[[[5-[[[3-(dimethylamino)propyl]amino]carbonyl]-3-thienyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]- (GA INDEX NAME)

L10 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

(Continued)

PAGE 1-A

L10 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2005 ACS on STM (Continued)
REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 13 Sep 2001
AB The solution-phase, parallel synthesis and evaluation of a library of 132
(+)-1,2,9,9a-tetrahydrocyclopropa[c]benz[e]indol-4-one (CBI) analogs of
CC-1065 and the duocarmycins containing dimeric monocyclic, bicyclic, and
tricyclic heteroarom replacements for the DNA-binding domain are
described. This systematic study revealed clear trends in the structural
requirements for observation of potent cytotoxic activity and DNA
alkylation efficiency, the range of which spans a magnitude of 210
000-fold. Combined with related studies, these results highlight that the
role of the DNA-binding domain goes beyond simply providing DNA-binding
selectivity and affinity (10-100-fold enhancement in properties),
consistent with the proposal that it contributes significantly to
catalysis of the DNA alkylation reaction accounting for as much as an
addn1 1000-fold enhancement in properties).
ACCESSION NUMBER:
2001:667407 CAPLUS
DOCUMENT NUMBER:
2001:667407 CAPLUS
DOCUMENT NUMBER:
201:667407 CAPLUS
DOCUMENT NUMBER:
201:667407 CAPLUS
DOCUMENT NUMBER:
201:667407 CAPLUS
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207:667407 CAPLUS
DOCUMENT HORDER:
208:67407 CAPLUS
DOCUMENT HORDER:
209:667407 CAPLUS
DOCUMENT HORDER:
200:667407 English CASREACT 135:357786 LANGUAGE: OTHER SOURCE(S): IT 372953-56-5P 372933-56-59
RL: ADV (Adverse effect, including toxicity): BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SFN (Synthetic preparation): BIOL (Biological study): PREP (Preparation) (synthesis and evaluation of tetrahydrocyclopropa(c)benz[e]indol-4-one analogs of CC-1065 and the duocarmycins defining the contribution of the DNA-binding domain)
372953-56-5 CAPLUS
Carbamic acid, [5-[[[S-[[(IS)-1-(chloromethyl)-1,2-dihydro-5-hydroxy-3H-benz[e]indol-3-yl]carbonyl]-3-thienyl]amino[carbonyl]-1-methyl-1H-pyrrol-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 27 Jul 2001

AB The title compds. [I: X = 0, S: Rl = alkyl, cycloalkyl, halo: R2 = H, alkyl, alkoxy, etc.: R3 = alkyl: A = (un)substituted ortho-substituted (hetero)aryl, bicyclo(hetero)aryl) which have plant-protective properties and are suitable for protecting plants against infestations by phytopathogenic microorganisms, were prepared Thus, methylation of Me 4-methylpyrrole-3-carboxylate followed by hydrolysis of the resulting ester, and reaction of 1,4-dimethylpyrrole-3-carboxylic acid with 2-(4'-fluorophenyl)anilne afforded I [X = 0: Rl, R3 = Me: R2 = H: R = 4'-fluorobiphenyl-2-yl] which showed strong efficacy against Puccinia recondita on wheat (< 206 infestation).

ACCESSION NUMBER: 2001:545661 CAPLUS
DOCUMENT NUMBER: 135:137397

TITLE: Preparation of pyrrolecarboxamides and pyrrolecthioamides as fungicides
INVENTOR(S): Syngent Participations A.-G., Switz.

PATENT ASSIGNEE(S): Syngent Participations A.-G., Switz.

POT Int. Appl., 111 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

DOCUMENT TYPE:

English FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA	TENT	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D	ATE	
						-									-		
WO	200	10532	59		A1		2001	0726		WO 2	001-	EP59	2		2	0010	119
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		CR,	CU,	CŽ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,
		ΗU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,
		LU,	LV,	MA,	MD,	MG,	MK.	MN,	MW,	MCX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,
		SD,	SE,	SG,	SI,	SK,	ŞĹ,	ΤJ,	TM,	TR,	TT,	TZ,	UΑ,	UG,	US,	UZ,	VN,
		YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	ŤJ,	TM				
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		DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
		ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
CA	2397	7008			AA		2001	0726		CA 2	001-	2397	008		2	0010	119
BR	200	10077	38		A		2002	1022		BR 2	001-	7738			2	0010	119
EP	1252	2140			A1		2002	1030		EP 2	001-	9074	68		2	0010	119
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR						
		35202														0010	119
AU	7720	535			B2		2004	0506		AU 2	001-	3543	3		2	0010	119
ZA	2002	20056	41		A		2003	1103		ZA 2	002-	5641			2	0020	715
US	2004	10490								US 2	002-	1817	02		2	0021	800
US	680	5286			В2		2004	1019									

(Continued) 20031007 A 20000121 W 200101 US 2002-181702 A3 2002108

OTHER SOURCE(s): MARPAT 135:137397

IT 351416-74-5P 351416-75-6P 351416-76-7P

R1: AGR (Agricultural use): BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SPN (Synthetic preparation): BIOL (Biological study): PREP (Preparation): USES (Uses)

(preparation of pyrrolecarboxamides and pyrrolethioamides as fungicides)

RN 351416-74-5 CAPLUS

CN 1H-Pyrrole-3-cachoxamide, N-[2-(4-chlorophenyl)-3-thlenyl]-1,4-dimethyl
(9C1) (CA INDEX NAME) US 2002-181702

351416-75-6 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-1-methyl-4(pentafluoroethyl)- (9CI) (CA INDEX NAME)

351416-76-7 CAPLUS 1H-Pyrrole-3-carboxamide, N-[2-(4-fluorophenyl)-3-thienyl]-1-methyl-4-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 13 Jul 2001 $_{\rm GI}$

AB The title compds. [I; X = 0, S; Rl = H, alkyl, halo; R2 = alkyl; A = ortho-substituted aryl, ortho-substituted heteroaryl, bicycloaryl, bicycloheteroaryl] which have plant-protective properties and are suitable for protecting plants against infestations by phytopathogenic microorganisms, were prepared E.g., a multi-step synthesis of I [Rl = H; R2 = Me; X = 0; A = 4-(4-chlorophenyl)pyridin-3-yl] which showed strong efficacy against Erypsiphe graminis on barley, was given.

ACCESSION NUMBER: 2001:50767 CAPLUS
DOCUMENT NUMBER: 135:92339

TITLE: representation of trifluoromethylpyrrole carboxamides and trifluoromethylpyrrole biographs as functioned.

135:92539
Preparation of trifluoromethylpyrrole carboxamides and trifluoromethylpyrrolethioamides as fungicides Walter, Harald; Trah, Stephan; Schneider, Hermann Syngenta Participations A.-G., Switz.
PCT Int. Appl., 65 pp.
CODEN: PIXXD2
Patent INVENTOR(S): PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE:

English FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PATENT NO.														D	ATE		
	2001							0712			2000-				2	0001	111	
											BG,							
											FI,							
											KR,							
		LU,	LV,	MA,	MD,	MG.	MK,	MN,	MW.	MX,	MZ,	NO.	NZ,	PL.	PT.	RO.	RU,	
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		YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM					
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BR	2000	0168	71		А		2002	1008		BR 2	2000-	1687	1		2	0001	111	
EP	1252																	
	R:										IT,	LI,	LU,	NL,	SE,	MC,	PT,	
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	2003																	
EG	2259	9			A		2003	0430		EG 2	2000-	1588			2	0001	224	
ZA	2002	0048	74		А		2003	0918		ZA 2	2002-	4874			2	0020	618	
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	2004				A1		2004	0902			2004-							
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										us z	2002-	1692	81		A3 2	0021	800	

L10 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN OTHER SOURCE(S): MARPAT 135:92539 IT 349466-95-9P 349486-96-0P 349486-97-1P 349465-98-2P (Continued)

349486-98-2P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of trifluoromethylpyrrole carboxamides and trifluoromethylpyrrolethioamides as fungicides)
349486-95-9 CAPLUS

1H-Pyrrole-3-carboxamide, 1-methyl-N-[2-(4-methylcyclohexyl)-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

349486-96-0 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(4-isoxazoly1)-3-thieny1]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

349486-97-1 CAPLUS
1H-Pyrcole-3-carboxamide, N-{2-{3-fluoro-4-pyridinyl}-3-thienyl}-1-methyl-4-ttrifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

349486-98-2 CAPLUS
1H-Pyrrole-3-carboxamide, N-{2-{1,2-dihydro-2-oxo-3-pyridinyl}-3-thienyl}-1-methyl-4-{trifluoromethyl}- (9CI) (CA INDEX NAME)

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)

DX, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,

CA 2355734 AA 20000810 CA 2000-22355734 20000131

BR 2000008015 A 200101106 BR 2000-8015 20000131

FI 173421 A2 20020123 PF 2000-901747 20000131

R: AT, BE, CH, DE, DX, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

IE, SI, LT, LV, FI, RO

JP 200253652 T2 2002029 JP 2000-597270 20000131

NO 2001003766 A 20011001 NO 2001-3768 20106619

NO 2001003768 A 20011001 NO 2001-3768 20106019

PRIORITTY APPLIN. INFO::

GB 1999-2455 A 19990205

PRIORITTY APPLIN. INFO::

W 2000-668284 W 20000131

OTHER SOURCE(s): MARPAT 133:150463

IT 287725-88-6P

R1: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological atudy); PREP (Preparation); USES (Uses) (preparation of 3-substituted indole-2-carboxylic acids for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis)

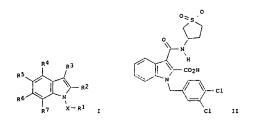
RN 287725-88-6 CAPIUS

CN 1H-Indole-2-carboxylic acid, 1-((3,4-dichlorophenyl)methyl)-3-([(teraphydro-1,1-dioxido-3-thienyl)amino)carbonyl)- (9CI) (CA INDEX NAME)

287726-47-0P

287726-47-09
RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of 3-substituted indole-2-carboxylic acids for the inhibition
of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis)
287726-47-0 CAPLUS
1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3[(tetrahydro-1,1-dioxido-3-thienyl)amino]carbonyl]-, ethyl ester (9CI)
(CA INDEX NAME)

ANSWER 16 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 11 Aug 2000



AB The title compds. [1; X = CH2, SO2; R1 = (un)substituted aryl, heteroaryl; R2 = CO2H, CN, COCH2OH, etc.; R3 = OR15 (wherein R15 = substituted alkyl or cycloalkyl, (un)substituted heteroaryl), S(O)qR15 (q = O-2), (CH2)aCO2H (s = O-4), etc.; R4-R7 = H, (un)substituted hydrocarbyl, heterocyclyl, etc.) and their pharmaceutically acceptable salts, amides or esters, useful in the preparation of a medicament for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis, were prepared and formulated. Thus, hydrolysis of the corresponding ester afforded 93% II which showed 1C50 of 6.6 µM against hMCP-1 receptor binding. ACCESSION NUMBER: 2000:553556 CAPLUS 2000:UMENT NUMBER: 133:150463 Preparation of 3-substituted indole-2-carboxylic acids for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis Protein-1 and/or RANTES

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	ENT I	NO.			KIN	D	DATE			APPL	I CAT	ION	NO.		D.	ATE	
						-									-		
WO	2000	0461	99		A2		2000	0810	,	WO 2	000-	GB28	4		2	0000	131
WO	2000	0461	99		A3		2000	1130									
	W:	ΑE,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU
		CZ,	DE,	DK,	DM,	ĒE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	ΗU,	ID,	ΙL
		IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA
		MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI
		SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UŻ,	VN,	YU,	ZA,	ZW,	AM
		AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM								
	RW:	GH,	GM,	KE.	LS.	MW.	SD.	SL.	SZ.	TZ.	UG.	ZW.	AT.	BE.	CH.	CY.	DE

L10 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

ANSWER 17 OF 22 CAPLUS COPYRIGHT 2005 ACS ON STN Entered STN: 20 Jun 2000

AB The development of a solution-phase synthesis of distamycin A and its extension to the preparation of 2640 analogs are described. Thus, solution-phase synthesis techniques with reaction workup and purification employing acid/base liquid-liquid extns. were used in the multiatep preparation of distamycin A (8 steps, 400 overall yield) and a prototypical library of 2640 analogs providing intermediates and final products that are 295% pure on conventional reaction scales. The complementary development of a simple, rapid, and high-throughput screen for DNA binding affinity based on the loss of fluorescence derived from displacement of prebound echidium bromide is disclosed which is applicable for assessing relative or absolute binding affinity to DNA homopolymers or specific sequences (hairpin oligonucleotides). Using hairpin oligonucleotides, this method permits the screening of a library of compds. against a single predefined sequence to identify high affinity binders, or the screening of a single compound against a full library of individual hairpin oligonucleotides to define its sequence selectivity. The combination permits the establishment of the complete DNA binding profile of each member of a library of compds. Screening the prototypical library provided compds. that are 1000 times more potent than distamycin A in cytotoxic assays [1, Boc = tert-butoxycarbonyl: IC50 = 29 nM, IL210), that bind to poly[dA]-poly[dT] with comparable affinity, and that exhibit an altered DNA binding sequence selectivity. Several candidates were identified which bound the

L10 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(dimethylamino)-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]2-thienyl]carbonyl]-3,6,7,8-tetrahydro-, methyl ester (9CI) (CA INDEX

292070-05-4P 292071-72-8P

292070-05-49 292071-72-89 RE: RCT (Reactant); PREP (Preparation); RACT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (total synthesis of distamycin A and solution-phase combinatorial approach to distamycin A analogs as DNA binding agents) 292070-05-4 CAPLUS (Preparation) (Preparation) 272070-05-4 CAPLUS (Preparation) (Prep

292071-72-8 CAPLUS
2-Thiophenecarboxylic acid, 4-{{{4-{{(1,1-dinethoxylcarbonyl}amino}-1-methyl-1H-pyrrol-2-yl]carbonyl}amino}-2-thienyl]carbonyl]amino}-, methyl ester (9CI) (CA INDEX NAME)

L10 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
five-base-pair AT-rich site of the PSA-ARE-3 sequence, and one (II, R =
4-dimethylaminobutyryl; K = 3.2 + 106 M-1) maintained the high
affinity binding (K = 4.5 + 106 M-1) to the ARE-consensus sequence
contg. a GC base-pair interrupted five-base-pair AT-rich site suitable for
inhibition of gene transcription initiated by hormone insensitive androgen
receptor dimerization and DNA binding characteristic of therapeutic
resistant prostate cancer.

ACCESSION NUMBER: 2000:405663 CAPLUS
DOCUMENT NUMBER: 133:223039
TOTAL Synthesis of Distamycin A and 2640 Analogs: A
Solution-Phase Combinatorial Approach to the Discovery
of New, Bioactive DNA Binding Agents and Development
of a Rapid, High-Throughput Screen for Determining
Relative DNA Binding Affinity or DNA Binding Sequence
Selectivity

Relative DNA Binding Affinity or DNA Binding Sequence Selectivity
Boger, Dale L.: Fink, Brian E.: Hedrick, Michael P. Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA Journal of the American Chemical Society (2000), 122(27), 6382-6394 CODEN: JACSAT; ISSN: 0002-7863 American Chemical Society Journal English CASREACT 133:223039 337-59 AUTHOR(S): CORPORATE SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

SOURCE:

LANGUAGE:

English
OTHER SOURCE(S): CASREACT 133:223039

T1 292069-27-3P 292069-37-5P

R1: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified): SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(total synthesis of distamycin A and solution-phase combinatorial approach to distamycin A analogs as DNA binding agents)

RN 292069-27-3 CAPLUS

CN Benro[1,2-b:4,3-b')dipyrrole-2-carboxylic acid, 6-[[4-[[[4-([(1,1-dimethyl=thoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-2-thienyl]carbonyl]-3,6,7,8-tetrahydro-, methyl ester (9CI) (CA INDEX NAME)

292069-37-5 CAPLUS Benzo[1,2-b:4,3-b']dipyrrole-2-carboxylic acid, 6-[{4-[{4-[{4-

L10 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 18 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 25 Feb 2000

AB Title compds. I (Rl = H, halo, alkyl, haloalkyl; R2 = alkyl, haloalkyl, alkoxyalkyl, cyano, alkylsulfonyl, arylsulfonyl, etc.: A = substituted Ph, substituted 3-thienyl, substituted 4-indanyl) were prepared as plant protectants. Thus, 1.9 g l-methyl-4-(trifluoromethyl)pyrrole-3-carboxylic acid, obtained from Et 4.4-trifluorocrotonate, tosylmethyl isocyanide, and MeI, and 0.9 mL oxalyl chloride in 20 mL CH2Cl2 was stirred at room temperature in the presence of a catalytic amount of DMF, the solvent was evaporated under reduced pressure to give a crystalline solid, and the solid was added to a solution of 1.7 g of 2-biphenylamine and 4.2 mL Bt3N in 20 mL CH2Cl2 at 0°, and the reaction mixture was stirred for 2 h at room temperature to give I (Rl = H, R2 = Me, A = 2-biphenylyl). Application of this compound on apples, grapes, and tomatoes resulted in <10% infestation by Botrytis cinerea.

ACCESSION NUMBER: 2000:133660 CAPLUS

ACCESSION NUMBER:
DOCUMENT NUMBER:
TITLE:
INVENTOR(S):
PATENT ASSIGNEE(S):

2000:133660 CAPPUS
132:166122
(Trifluoromethyl)pyrrolecarboxamides
Eberle, Martin: Walter, Harald
Novartis A.-G., Switz.; Novartis-Erfindungen
Verwaltungsgesellschaft m.b.H.
PCT Int. Appl., 35 pp.
CODEN: PIXXD2
Patent

SOURCE:

DOCUMENT TYPE: Patent English COUNT: 1 FAMILY ACC. NUM. CO PATENT INFORMATION

	TENT				KIN	D	DATE					ION			D.	ATE	
	-					-									-		
WO	2000	0094	82		Al		2000	0224	1	WO 1	999-	EP58	37		1	9990	810
	W:	ΑE,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,
		CZ,	DE,	DK,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,
		IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,
		MK.	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,
		TJ,	TM,	TR,	TT,	UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,
		KZ,	MD,	RU,	TJ.	TM											
	RW:	GH,	GM,	KE,	LS,	MW,	SD,	SL,	SZ,	UG,	ZW.	AT,	BE,	CH,	CY,	DE,	DK,
		ES,	FI.	FR.	GB.	GR,	IE,	IT.	LU,	MC,	NL,	PT.	SE,	BF.	BJ,	CF,	CG,
		CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG					
TW	5768	31			В		2004	0221		TW 1	999-	B810	7745		1	9990	513
ΑU	9955	138			A1		2000	0306		AU 1	999-	5513	8		1	9990	810
ΑU	7561	40			B2		2003	0102									
BR	9912									BR 1	999-	1296	2		1	9990	810
	1105																
							ES,								_		

L10 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 18 OF 22	CAPLUS CO		005 A	CS on STN	(Conti	nued)
TR 200100478	т2	20010621	TR	2001-20010047	В	19990810
JP 2002522526	T2	20020723	JP	2000-564936		19990810
US 2002019541	A1	20020214	US	2001-780897		20010209
US 6365620	B2	20020402				
PRIORITY APPLN. INFO.:			GB	1998-17548	A	19980812
			WO	1999-EP5837	W	19990810
OFFICE COURCE (C) .	MADDAT	122.16612	2			

OTHER SOURCE(S): MARPAT 132:166122

IT 258510-89-29 258510-89-39 258510-91-79

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study); PREP (Preparation)

((trifluoromethyl)pytrolecarboxamides as plant protectants)

RN 258510-88-2 CAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[2-(4-fluorophenyl)-3-thienyl]-1-methyl-4
(trifluoromethyl)- (9CI) (CA INDEX NAME)

258510-89-3 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

258510-91-7 CAPLUS HH-Pyrrole-3-carboxamide, N-(2-(1,1'-biphenyl]-4-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

ANSWER 19 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 08 Sep 1999

AB Indole derivs. (I) and (II) [where R1 = H, halogen, CF3, C1-10 alkyl, S-C1-10 alkyl, C1-10 alkoxy, CN, NO2, NN2, Ph, OPh, SPh, CH2Ph, OCH2Ph, SCN2Ph, or (un) substituted amido, carbamido, sulfonyl, etc.; R2 = H, halogen, CF3, CH, C1-10 alkyl, C1-10 alkoxy, CHO, CN, NO2, (un) substituted amino, SO2-C1-6 alkyl; R3 = (un) substituted carboxylic acid, OPO31A2, SO3H, etc.; R4 = H, CF3, C1-6 alkyl, C1-6 alkoxy, (C1-6 alkyl)-cycloalkyl, CHO, halogen, etc.; R5 = C1-6 alkyl, C1-6 alkoxy, (C1-6 alkyl)-cycloalkyl, etc.] and pharmaceutically acceptable salts thereof, were prepared by several methods. Thus, 5-nitroindole was C3-alkylated with Me 4-(bromomethyl)-3-methoxybenzoate in dioxane, N-alkylated with 1-iodopropane in a solution of THF and NaH, and converted to the amine by hydrogenation over Pt/C. The amine was converted to the carbamate by addition of cyclopentyl chloroformate in CH2C12 and 4-methylmorpholine and the resultant ester hydrolyzed to yield 4-(15-[(cyclopentyloxylcarbonyl]amino)-1-propyl-1H-indol-3-yl)methyl]-3-methoxybenzoic acid (III). The title compds are useful as phospholipase enzyme inhibitors, especially cytosolic phospholipase A2 (cPLAZ), for treatment of inflammatory conditions, particularly where inhibition of production of prostaglandins, leukotrienes, and PAF are all desired. Over one hundred compds of the invention were tested for cPLA2 inhibiting activity in the Coumarine assay and rat carragenan-induced footpad edema test. Compds. exhibited 71 to 981 inhibition at concns. of 0.125 µN to 400 µN in the Coumarine assay and -7.16 to 34.521 inhibition at concns. of 2 µM to 20 µM in the footpad edema test.

ACCESSION NUMBER: 1399:566026 CAPLUS
DOCUMENT NUMBER: 139:9:566026 CAPLUS
DOCUMENT NUMBER: 139:9:566026 CAPLUS
DOCUMENT NUMBER: 139:9:566026 CAPLUS
DOCUMENT NUMBER: 139:9:566026 CAPLUS John C. Loverine Protection of protection of indole derivatives as phospholipase enzyme inhibitors

131:199619
Preparation of indole derivatives as phospholipase
enzyme inhibitors
Seehra, Jasbir S.: McKew, John C.: Lovering, Frank;
Bemis, Jean E.: Xiang, Yibin: Chen, Lihren; Knopf,
John L. INVENTOR(S):

John L. Genetics Institute, Inc., USA PCT Int. Appl., 182 pp. CODEN: PIXXD2 Patent PATENT ASSIGNEE(S):

DOCUMENT TYPE: LANGUAGE: English

L10 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION: (Continued)

PATENT NO.																			
								WO 1999-US3898											
WO 9943654				A3 19991028															
	W:	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR	, BY	t. ·	CA,	CH,	CN,	cu,	CZ,	DE,	
		DK,	EE,	ES,	FI,	GB,	GĎ,	GE,	GH,	ĢΜ	, HF	٠.	HU,	ID,	IL,	IN,	IS,	JP,	
		KE.	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS	, LT	Γ,	LU,	LV,	MD,	MG,	MK,	MN,	
		MW,	MX.	NO,	NZ,	PL.	PT,	RO.	RU,	SD	. SE	٠.	SG.	SI.	SK,	SL,	TJ.	TM.	
		TR.	TT.	UA.	UG,	UZ.	VN,	YU.	ZW,	AM	. A2	٠.	BY.	KG.	KZ.	MD.	RU,	TJ,	TM
	RW:	GH,	GM.	KE.	LS.	MW.	SD.	52.	UG,	2W	. A1	r.	BE.	CH.	CY.	DE.	DK.	ES,	
		FI.	FR.	GB.	GR.	IÈ.	IT.	LU.	MC.	NL	. P1	r.	SE.	BF.	BJ.	CF.	CG.	CI.	
		CM,	GΑ,	GN,	GW,	ML,	MR,	NE,	SN,	TD	, TO	;							
CA	2322162			AA	AA 19990902				CA 1999-2322162 AU 1999-27825							19990224			
ΑU	9927	825			A1		1999	0915		ΑU	1999	9-2	782	5		1	9990	224	
ΑU	7654	27			B2		2003	0918											
BR	9908	275			А		2003 2000	1024		BR	1999	9-8	275			1	9990	224	
TR	2000	0244	7		T2		2000	1121		TR	2000)-2	0000	244	7	1	9990	224	
EP	1062	205			A2		2000	1227		EΡ	1999	9-9	083	78		1	9990	224	
							ES,												FI
JP	2002	5045	41		T2		2002			JP	2000	-5	334	12		1	9990	224	
EE	2000	0048	8		А		2002 2004	0215		EE	2000	-4	88			1	9990	224	
NZ	5063	29			A		2004	0130		ΝZ	1999	9-5	0632	29		1	9990	224	
NO	2000	0042	19		Α		2000	1023		NO	2000	-4	219			2	0000	823	
HR	2000	0005	51		A1		2001	0430		HR	2000	0-5	51			2	0000	824	
BG	1047	79			А		2001	1031		BG	2000) – 1	047	79		2	0000	919	
	APP																9980		
										WO	1999	9-U	S38	98		W 1	9990	224	
R 50	URCE	(S):			MARI	PAT	131:	1996	19										
241	497-	74-50	DP. e	ster	•														

241497-74-5P

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241497-74-5P
RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of indole derivs. as phospholipase enzyme inhibitors for treatment of inflammatory conditions)

ANSWER 20 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 03 Sep 1994

AB Title compds. I (R1 = MeCHMe, MeCHF, HOCH2; R2 = H, C1-4 alkyl; Z = HO2C, HO3S, tetrazol-5-yl, C1-4alkyl-SO2NHCO; A = (substituted)Ph or thienyl) a pharmaceutically acceptable salt or in vivo hydrolyzable ester thereof, are prepared 2-Thiophenecarboxylic acid was nitated to give the 4-nitro derivative, reduced ti the 4-amino derivative converted to the (25, 43)-1-(4-nitrobenzylcarbonyl)-2-(2-carboxy4-thienylcarbamoyl)pyrrolidin-4-ylthloacetate which in in 4 steps was converted to 58, 65, 88, 25, 43)-1 (R1 = MeCHOH, R2 = H, A = 4-thienyl. z = 2-HO2C) which had a min. inhibitory concentration of 0.5 mg/mL against Enterobacter cloacae 108 vs 32 mg/L of ceftriaxone. Pharmaceutical formulations comprising I are given.

ACCESSION NUMBER: 1994:508368 CAPLUS
DOCUMENT NUMBER: 1994:508368 CAPLUS
TITLE: Preparation of antibiotic pyrrolidinylthiopenem derivatives siret, Patrice Jean

INVENTOR(S): Siret, Patrice Jean

PATENT ASSIGNEE(S): Zeneca Ltd., UK; Zeneca Pharma S.A.

SOURCE: EXXDW

POCOUMENT TYPE: Patent

Patent

PATENT ASSIGNEE(S): English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 592167	Al	19940413	EP 1993-307843	19931001
EP 592167	Bl	19991222		
R: AT, BE, CH,	DE, DK,	ES, FR, GB,	GR, IE, IT, LI, LU,	MC, NL, PT, SE
CA 2106330	AA	19940408	CA 1993-2106330	19930916
AT 187968	Ε	20000115	AT 1993-307843	19931001
ES 2140445	Т3	20000301	ES 1993-307843	19931001
JP 06211871	A2	19940802	JP 1993-250437	19931006
US 5538962	A	19960723	US 1993-132256	19931006
PRIORITY APPLN. INFO.:			EP 1992-402733	A 19921007
OTHER SOURCE(S):	MARPAT	121:108368		
IT 155481-27-9P 155481-2	8-OP 15	6631-41-3P		
156631-42-4P				

(CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 241497-74-5 CAPLUS
CN 3-Thiophenecarboxylic acid, 4-[[[5-[(cyclopentylcarbonyl)amino]-1(diphenylmethyl)-1H-indol-3-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

L10 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

155481-28-0 CAPLUS
1-Pyrrolidinecarboxylic acid, 2-[[(5-carboxy-3-thienyl)amino]carbonyl]-4-mercapto-, 1-[(4-nitrophenyl)methyl] ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

156631-41-3 CAPLUS

Absolute stereochemistry.

L10 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
4-Thia-1-arabicyclo[3.2.0]hept-2-ene-2-carboxylic acid,
6-(1-hydroxyethyl)-3-[1-[(4-nitrophenyl)hethoxy]carbonyl]-5-[([5-{(2-propenyloxy)carbonyl}-3-thienyl]amino]carbonyl]-3-pyrrolidinyl]thio]-7-oxo, 2-propenyl ester, [SR-[3(35*,55*),5a,6a(R*)]]- (9CI) (CA

Absolute stereochemistry.

L10	ANSWER 21 OF 22	CAPLUS	COPYRIGHT 200		TO OR OTH	(Conti	nuad)
ы	AT 185140	E	19991015		1993-906740	(CONCI	19930324
	ES 2136124	T3	19991116		1993-906740		19930324
	CA 2108356	С	20040120		1993-2108356		19930324
	CN 1077957	A	19931103	CN	1993-102800		19930326
	CN 1036713	В	19971217				
	NO 9304264	А	19931125	NO	1993-4264		19931125
	FI 104075	B1	19991115	FI	1993-5245		19931125
	US 5519015	А	19960521	US	1993-142459		19931126
PRIO	RITY APPLN. INFO.	:		EP	1992-400836	А	19920326
				EP	1992-402763	A	19921009
					1993-GB603	A	19930324
OTHE	R SOURCE(S):	MARE	AT 121:9029			• • • • • • • • • • • • • • • • • • • •	
IT	155481-26-8P 155						
••	155481-30-4P 155						
	RL: RCT (Reactan				ation): PREP	Prenar	ation): RACT
	(Reactant or rea		(bymemetre pro	.pu.	acton,, that	, r r cpur	401011// 10101
			tion of, in p				
	oxythienylcarbamo	and read	tion or, in p	ера	racion or		
Calb							
	ylthiocarbape		xylates;				
RN	155481-26-8 CAP						
CN	1-Azabicyclo(3.2						
	thienyl)amino]ca					oonyl]-	3-
	pyrrolidinyl thi						
	2-[(4-nitropheny						
	R*)]]-, compd. w	ith N-et	hyl-N-(1-methy	/let	hyl)-2-propan	amine (1:1) (9CI)
	(CA INDEX NAME)						

CO₂H

CM 2 CRN 7087-68-5 CMF C8 H19 N

CM 1

CRN 155481-25-7 CMF C35 H33 N5 O13 S2

L10 ED GI ANSWER 21 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 09 Jul 1994

AB Title compds. I (R = (un)substituted carboxythienyl; Rl = CHNeOH, CHMeF, CHZOH; R2, R3 = H, alkyl] were prepared Thus, the carbapenem II was obtained from the diphenylphosphoryloxycarbapenem and the thiol, prepared from 2-thiophenecarboxylic acid and the protected mercaptopyrrolidinecarboxylic acid in 4 steps. II had mln. inhibitory concns. against Staphylococcus aureus Oxford 0.125 and Escherichia coli DCO 0.008 µg/mL. 1994:409029 CAPLUS
DCOUMENT NUMBER: 1994:409029 CAPLUS
DCOUMENT NUMBER: 121:9029
TITLE: Carbapenem derivatives as antibiotics and intermediates thereof

1994:409029 CAPLUS
121:9029
Carbapenem derivatives as antibiotics and intermediates thereof
Jung, Frederic Henri
Zeneca Ltd., UK: Zeneca Pharma S. A.
PCT Int. Appl., 44 pp.
CODEN: PIXXD2
Patent

INVENTOR(S):
PATENT ASSIGNEE(S):
SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA:	TENT	NO.			KIN	D D	ATE			APP	LI	CAT	ION	NO.		D.	ATE		
WO	9319	070			A1	1:	9931	0930		WO	19	93-	GB60	3		1	9930	324	
	W:	AT,	AU,	BB,	BG,	BR, G	CA,	CH,	CZ,	DΕ		DΚ,	ES,	FI,	GB,	HU,	JP,	KP,	
		KZ.	LK,	LU,	MG.	NL, I	NO,	PL,	RO										
	RW:	AT.	BE.	CH.	DE.	DK, I	ES.	FR.	GB.	GR		IE.	IT.	LU.	MC.	NL.	PT.	SE,	
						CI.													
ZA	9301	611			A	1	993	0927		ZA	19	93-	1611			1	9930	305	
II.	1051	35			A1	21	000	0131		IL	19	93-	1051	35		1	9930	323	
AU	9337	636			A1	1	993	1021		ΑU	19	93-	3763	6		1	9930	324	
AU	6629	72			B2	1	995	0921											
EP	5866	63			A1	1	994	0316		EР	19	93-	9067	40		1	9930	324	
EP	5866	63			B1	1	999	0929											
	R:	AT.	BE.	CH.	DE.	DK, I	ES.	FR.	GB.	GR		IE.	IT.	LI.	LU.	MC.	NL.	PT.	SE
ΗU						1													
						1											9930		
	2212				92											_			

L10 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

155481-27-9 CAPLUS
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[{5-carboxy-3-thienyl]amino]carbonyl]-, 1-[(4-nitrophenyl)methyl] ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

155481-28-0 CAPLUS 1-Pyrrolidinecarboxylic acid, 2-[[(5-carboxy-3-thienyl)amino]carbonyl]-4-mercapto-, 1-[(4-nitrophenyl)methyl] ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

155481-30-4 CAPLUS 155481-30-4 CAPLUS

1-Azabicyclo[3].2.0)hept-2-ene-2-carboxylic acid, 3-[[5-[[(2-carboxy-3-thienyl)amino]carbonyl]-1-[[(4-nitrophenyl)methoxy]carbonyl]-3-pyrrolidinyl]thio]-6-[1-hydroxyethyl]-4-methyl-7-oxo-, 2-[2-propenyl) ester, [4R-[3[38].55], 4a,5,6,6[R*]]]-, compd. with N-ethyl-N-(1-methylethyl)-2-propanamine (1:1) [9CI] (CA INDEX NAME)

CM 1

CRN 155481-29-1 CMF C31 H32 N4 O11 S2

Absolute stereochemistry.

CM 2 CRN 7087-68-5 CMF C8 H19 N

Et 1-Pr-N-Pr-1

155481-31-5 CAPLUS 133401313 Artis 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-{{(2-carboxy-3-thienyl)amino[carbonyl]-, 1-{(4-nitrophenyl)methyl) ester, (25-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

1-Pyrrolidinecarboxylic acid, 4-mercapto-2-[(3-thienylamino)carbonyl]-, (4-nitrophenyl)methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 29 Nov 1991

Title compds. I [R = 5- or 6-membered (monohydroxylated) (O- or S-containing) saturated cyclic amino, Q, Q1], useful for treatment of amnesia and dementia, are prepared Treatment of carbobenzoxyl-pyroglutamic acid with thiazolidine, 1-hydroxybenztriazole.HZO, and DCC in MeCN at room temperature

for 14 h gave N-(1-benzyloxycarbonyl-5-oxo-L-prolyl)thiazolidine, which inhibited prolyl endopeptidase with ICSO of 0.32 µM.

ACCESSION NUMBER: 1991:632874 CAPLUS
COCUMENT NUMBER: 115:232874

TITLE: Preparation of pyroglutamic acid amides as prolyl endopeptidase inhibitors
INVENTOR(S): Furukawa, Atsushi: Yoshimoto, Tadashi: Tsuru, Onori: Ajisawa, Yukiyoshi; Kinoshita, Yukihiko Kissei Pharmaceutical Co., Ltd., Japan Jpn. Kokai Tokkyo Koho, 7 pp.
CODENT TYPE: DOCUMENT TYPE: Patent JANGUAGE: Japanese

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

Japanese 1

PATENT NO. KIND DATE APPLICATION NO. DATE

Absolute stereochemistry.

L10 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L10 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

=> s 16

L11 2 L6

=> d ed abs ibib hitstr 1-2

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 27 Jul 2001

AB The title compds. [I; X = O, S: Rl = alkyl, cycloalkyl, halo; R2 = H, alkyl, alkoxy, etc.; R3 = alkyl; A = (un)substituted ortho-substituted (heterolaryl, bicyclo(heterolaryl) which have plant-protective properties and are suitable for protecting plants against infestations by phytopathogenic microorganisms, were prepared Thus, methylation of Me 4-methylpyrrole-3-carboxylate followed by hydrolysis of the resulting ester, and reaction of 1,4-dimethylpyrrole-3-carboxylic acid with 2-(4'-fluorobiphenyl)aniline afforded I [X = O: Rl, R3 = Me: R2 = H; A = 4'-fluorobiphenyl-2-yl] which showed strong efficacy against Puccinia recondita on wheat (< 20% infestation).

ACCESSION NUMBER: 2001:545661 CAPLUS
DOCUMENT NUMBER: 135:137397
Preparation of pyrrolecarboxamides and pyrrolethioamides as fungicides
INVENTOR(S): Walter, Harald: Schmeider, Hermann
Syngenta Participations A.-G., Switz.

PCT Int. Appl., 111 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION

PA'	FENT .				KIN	D	DATE								D	ATE	
						-											
WO	2001	0532	59		A1		2001	0726		WO 2	001-	EP59	2		2	0010	119
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		CR,	CU,	CZ,	DE,	DK,	DM,	DZ.	EE.	ES,	FI,	GB,	GD,	GE.	GH,	GM,	HR.
							JP,										
		LU.	LV.	MA.	MD.	MG.	MK,	MN.	MW.	MX.	MZ.	NO.	NZ.	PL.	PT.	RO.	RU.
							SL,										
							BY,									,	
	RW:						MZ,							AT.	BE.	CH.	CY.
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CP	2397															0010	119
	2001																
	1252																
LF																	
	к:						ES,					LI,	LU,	NL,	SE,	MC,	Pr,
							RO,										
JP	2003	5202	69		Т2		2003	0702		JP 2	001-	5532	63		2	0010	119
ΑU	7726	35			B2		2004	0506		AU 2	001-	3543	3		2	0010	119
ZA	2002	0056	41		А		2003	1103		ZA 2	002-	5641			2	0020	715

L11 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
US 2004049035 A1 20040311 US 2002-181702 20
US 6806286 B2 20041019 20021008 US 2003-680346 US 2004106521 20040603 20031007 GB 2000-1447 WO 2001-EP592 US 2002-181702 PRIORITY APPLN. INFO.: 20000121 20010119 A3 20021008

OTHER SOURCE(S): MARPAT 135:137397

IT 35:416-74-5P 35:416-75-6P 35:416-76-7P
R1: AGR (Agricultural use): BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SPN (Synthetic preparation): BIOL (Biological study): PREP (Preparation): USES (Uses)

(preparation of pyrrolecarboxamides and pyrrolecthioamides as fungicides)

RN 35:416-74-5 CAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-1,4-dimethyl(9CI) (CA INDEX NAME)

351416-75-6 CAPLUS 1H-Pyrrole-3-carbox

HH-Pyrrole-3-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-1-methyl-4-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

CAPLUS

1H-Pyrrole-3-carboxamide, N-[2-(4-fluorophenyl)-3-thienyl]-1-methyl-4-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 25 Feb 2000 GI

AB Title compds. I (RI = H, halo, alkyl, haloalkyl; R2 = alkyl, haloalkyl, alkoxyalkyl, cyano, alkylsulfonyl, arylsulfonyl, etc.: A = substituted Ph, substituted 3-thienyl, substituted 4-indanyl) were prepared as plant protectants. Thus, 1.9 g l-methyl-4-(trifluoromethyl)pyrrole-3-carboxylic acid, obtained from Et 4,4,4-trifluorocrotonate, tosylmethyl isocyanide, and MeI, and 0.9 mL oxalyl chloride in 20 mL CH2C12 was stirred at room temperature in the presence of a catalytic amount of DMF, the solvent was evaporated

evaporated
under reduced pressure to give a crystalline solid, and the solid was added to
a solution of 1.7 g of 2-biphenylamine and 4.2 mL Et3N in 20 mL CH2Cl2 at
0°, and the reaction mixture was stirred for 2 h at room temperature to
give I (R1 = H, R2 = Me, A = 2-biphenyly1). Application of this compound on
apples, grapes, and tomatoes resulted in <10% infestation by Botrytis
cinerea.
ACCESSION NUMBER: 2000:133660 CAPLUS

DOCUMENT NUMBER: TITLE: INVENTOR(S):

2000:133500 CAPUS
132:165122
(Trifluoromethyl)pyrrolecarboxamides
Eberle, Martin; Walter, Haraid
Novartis A.-G., Switz.; Novartis-Erfindungen
Verwaltungsgesellschaft m.b.B.; PATENT ASSIGNEE (S):

SOURCE: PCT Int. Appl., 35 pp. CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

DATE 20000224 APPLICATION NO. PATENT NO. KIND DATE A1 WO 1999-EP5837 19990810 WO 2000009482

TW 576831 AU 9955138 AU 756140 EP 1105375 A1 20010508 BR 1999-12962 19990810
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, UF, FI, RO
TR 200100478 T2 20010621 TR 2001-200100476

Lll	ANSWER 2 OF 2 CA	PLUS COR	YRIGHT 2005	ACS	on STN (Continue	1)
	JP 2002522526	T2	20020723	JP	2000-564936		19990810
	US 2002019541	Al	20020214	US	2001-780897		20010209
	US 6365620	B2	20020402				
PRIO	RITY APPLN. INFO.:			GB	1998-17548	A 1	9980812
				WO	1999-EP5837	w	9990810
отне	R SOURCE(S):	MAR PA1	132:166122				
IT	258510-88-2P 25851	0-89-3P 2	58510-91-7P				
	RL: BAC (Biologic	al activi	ty or effec	tor,	except adver	se); BSU	(Biologic
	study, unclassifi						
	study); PREP (Pre	paration)					
	((trifluoromet	hyl)pyrrc	lecarboxami	des a	as plant prot	ectants)	
RN	258510-88-2 CAPL	US					
	1H-Pyrrole-3-carb	oxamide.	N-[2-(4-flu	oropi	henyl)-3-thie	nyl]-1-me	thyl-4-
CN							

RN 258510-89-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-(4-chlorophenyl)-3-thienyl}-1-methyl-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 258510-91-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-[1,1'-biphenyl)-4-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

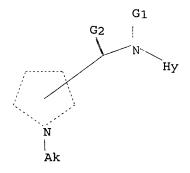
L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

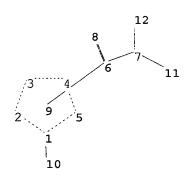
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Page 4230/08/2005

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	124.40	612.04
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-18.25	-18.25

STN INTERNATIONAL LOGOFF AT 12:06:27 ON 30 AUG 2005





chain nodes:
6 7 8 10 11 12
ring nodes:
1 2 3 4 5
chain bonds:
1-10 6-7 6-8 7-11 7-12
ring bonds:
1-2 1-5 2-3 3-4 4-5
exact/norm bonds:

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-12

G1:H,CH3

G2:0,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:Atom 12:CLASS Generic attributes :

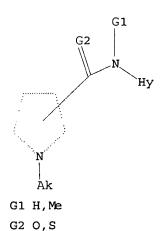
11:

Number of Carbon Atoms : less than 7 Number of Hetero Atoms : less than 2 Type of Ring System : Monocyclic

STR

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 S



Structure attributes must be viewed using STN Express query preparation.

=> s l1 SAMPLE SEARCH INITIATED 13:44:46 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 136055 TO ITERATE

1.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

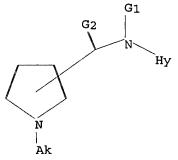
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 2699331 TO 2742869

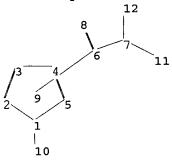
PROJECTED ITERATIONS: 2699331 TO 2742869
PROJECTED ANSWERS: 8214 TO 10832

L2 7 SEA SSS SAM L1

=>

Uploading C:\Program Files\Stnexp\Queries\10680346exp2.str





7 ANSWERS

chain nodes :
6 7 8 10 11 12
ring nodes :
1 2 3 4 5
chain bonds :
1-10 6-7 6-8 7-11 7-12
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-12

G1:H,CH3

G2:0,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS

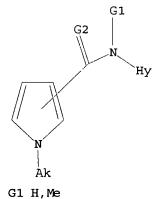
11:Atom 12:CLASS Generic attributes :

11:

Number of Carbon Atoms : less than 7 Number of Hetero Atoms : less than 2 Type of Ring System : Monocyclic

L3 STRUCTURE UPLOADED

=> d 13 L3 HAS NO ANSWERS L3 STR



G2 0, S

Structure attributes must be viewed using STN Express query preparation.

7 ANSWERS

=> s 13

SAMPLE SEARCH INITIATED 13:46:21 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 136055 TO ITERATE

1.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

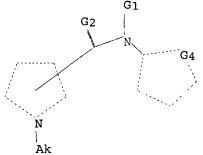
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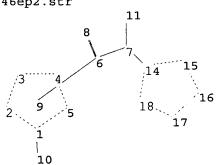
PROJECTED ITERATIONS: 2699331 TO 2742869 PROJECTED ANSWERS: 8214 TO 10832

L4 7 SEA SSS SAM L3

=>

Uploading C:\Program Files\Stnexp\Queries\346ep2.str





chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 15 16 17 18

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-15 14-18 15-16 16-17 17-18

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-15 14-18 15-16 16-17 17-18

G1:H,CH3

G2:0,S

G3:0,N

G4:0,S,N

Match level :

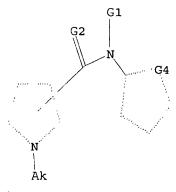
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



G1 H,Me

G2 0,S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 13:52:22 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1828 TO ITERATE

100.0% PROCESSED 1828 ITERATIONS

11 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

33996 TO 39124

PROJECTED ANSWERS:

22 TO 418

L6

L7

11 SEA SSS SAM L5

=> s 15 full

FULL SEARCH INITIATED 13:52:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 37137 TO ITERATE

100.0% PROCESSED 37137 ITERATIONS

294 SEA SSS FUL L5

294 ANSWERS

SEARCH TIME: 00.00.01

=> fil hcaplus COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST 166.92 167.13

FILE 'HCAPLUS' ENTERED AT 13:52:44 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 17 L8 41 L7

=> d ed abs ibib hitstr 1-41

ANSWER 1 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 13 May 2005

Title compds. I [wherein R1 = (un)substituted (C3-7 cycloalkyl)methyl, hetero/aryl; R2 = H, NO2, CN, CO2H and derivs., NH2 and derivs., etc.; R3 = (un)substituted hetero/aryl; and their pharmaceutically acceptable salts] were prepared as p38 MAP kinase inhibitors for treating and/or preventing immune or inflammatory disorders. For example, II was prepared by reacting Et 3-bromo-6-oxo-7-phenyl-6,7-dihydrothieno(2,3-b)pyridine-2-carboxylate (preparation given) with 3-methylbenzaldehyde and oxidation with

MnO2. I are potent inhibitors of p38 MAP kinase (IC50 around 2 µM and below),
especially p38c kinase.

ACCESSION NUMBER: 2005:409526 HCAPLUS

DOCUMENT TYPE: PATENT ASSIGNEE(S): SOURCE: PCT Int. Appl., 181 pp.
CODENT TYPE: PATENT ASSIGNEE(S): PCT Int. Appl., 181 pp.
CODENT TYPE: PATENT ASSIGNEE(S): PCT Int. Appl., 181 pp.
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CODENT TYPE: PATENT ASSIGNEE(S): PCT Int. Appl., 181 pp.
CODENT PCT INT. PATENT ASSIGNEE(S): PCT INT. PATENT ASSIG

FAMILY ACC. NUM. COUNT:

ANSWER 1 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

851753-37-2P, N-(3-Benzoyl-6-oxo-7-phenyl-6,7-dihydrothieno(2,3-b)pyridin-2-yl)-1-methyl-2-pyrrolidinecarboxamide 851753-40-7P, N-(3-Benzoyl-6-oxo-7-phenyl-6,7-dihydrothieno(2,3-b)pyridin-2-yl)-1-methyl-D-prolinamide RL: PAC (Fharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Uses)

(p38a kinase inhibitor: preparation of thienopyridinones as p38 MAP

kinase inhibitors useful in the treatment of and/or prevention of
immune or inflammatory disorders)

851753-37-2 MCAPBUS

2-Pyrrolidinecarboxamide, N-(3-benzoyl-6,7-dihydro-6-oxo-7phenylthieno[2,3-b]pyridin-2-yl)-1-methyl-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

851753-40-7 HCAPLUS
2-Pyrrolidinecarboxamide, N-(3-benzoyl-6,7-dihydro-6-oxo-7-phenylthieno[2,3-b]pyridin-2-yl)-1-methyl-, (2R)- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

L0 ANSWER 1 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN PATENT INFORMATION: (Continued)

PA1	ENT	NO.			KIN	D	DATE			APPL	ICAT	ION :	NO.		D.	ATE	
						-									-		
WO	2005	0425	40		A1		2005	0512	1	WO 2	004-	3B44	90		2	0041	022
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		CN,	co,	CR.	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GΕ,	GH,	GM,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	ΚŻ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	ΜA,	MD,	MG,	MK,	MN,	MW,	ΜX,	MZ,	NΑ,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	sc,	SD,	SE,	SG,	SK,	SL,	SY,
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	ŲĢ,	ZM,	ZW,	AM,
		ΑZ,	BY,	KG,	ΚŻ,	MD,	RU,	TJ,	TM.	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	ΒJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	G₩,	ML,	MR,	NE,
		SN,	TD,	TĢ													

PRIORITY APPLN. INFO.:

GB 2003-24902 GB 2003-29490 GB 2004-2918 GB 2004-16934

OTHER SOURCE(S): MARPAT 142:463710

THER SOURCE(S): MARPAT 142:463710

S51749-00-3P, tert-Butyl (2S)-2-{[(3-benzoyl-6-oxo-7-phenyl-6, 7-dihydrothieno[2,3-b]pyridin-2-yl)amino]carbonyl]pyrrolidine-1-carboxylate 851749-02-5P, tert-Butyl (2R)-2-{[(3-benzoyl-6-oxo-7-phenyl-6, 7-dihydrothieno[2,3-b]pyridin-2-yl)amino]carbonyl]pyrrolidine-1-carboxylate RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

[(Intermediate: preparation of thienopyridinones as p38 MAP kinase inhibitors useful in the treatment of and/or prevention of immune or inflammatory disorders)

RN 851749-00-3 HCAPLUS

N 1-Pyrrolidinecarboxylic acid, 2-{[(3-benzoyl-6,7-dihydro-6-oxo-7-phenylthieno[2,3-b]pyridin-2-yl)amino]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

851749-02-5 HCAPLUS
1-Pyrrolidinecarboxylic acid, 2-{{{3-benzoyl-6,7-dihydro-6-oxo-7-phenylthieno(2,3-b]pyridin-2-yl)amino}carbonyl}-, 1,1-dimethylethyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 1 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 06 Aug 2004

Condensed pyridines and pyrimidines (quinolines, quinazolines and thienopyrimidines) of formula I [X is N or CH: Y is -NR- or -NHCH2-; R is alkyl: A is a fused 5-7 membered carbocyclic or N/O/S-heterocyclic ring with one or more RI groups; RI is H, halo, NOZ, alkyl, OR, CONRAR5, O(CH2)nNRAR5, or NRAR5; R2 is certain N-containing heterocyclic rings; R3 is pyridin-2-yl, CI-6alkyl-pyridin-2-yl, -pyrrol-2-yl or -thiazol-2-yl; R4 is H or alkyl; R5 is alkyl: NRAR5 can be 3-7 membered (un)saturated N/O/S-heterocycle] and their pharmaceutically acceptable salts, solvates or derivs. were synthesized. Thus, 2-aminobenzamide was coupled with 6-methyl-2-pyridinecarboxylic acid in the presence of EDCI/HOBT followed by cyclocondensation mediated by NaOH to give quinazolinone II. Chlorination of II with POCI3 and subsequent substitution of the resulting chloride with 4-aminopyridine afforded quinazoline III. These compds. are inhibitors of the transforming growth factor TGF-P, especially of activin-like kinase ALK-5 receptor, and are used in the treatment and prevention of Various disease states mediated by ALK-5 kinase mechanisms such as kidney fibrosis. All the final products showed ALK5 receptor modulator activity with ICSO of 0.001-10 µM (82 nM for III) and TGF-P cellular activity with ICSO of 0.001-10 µM (82 nM for III). The role of ALK5 inhibitors for the treatment of photoaging was also demonstrated exptl. expt1. ACCESSION NUMBER:

2004:633933 HCAPLUS 141:174181

Preparation of quinolines, quinazolines and thienopyrimidines as ALK-5 receptor ligands for the treatment of kidney fibrosis Dodic, Nerina; Gellibert, Francoise Jeanne; Hunter,

DOCUMENT NUMBER:

INVENTOR (S):

ANSWER 3 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 19 Jul 2004

AB Hairpin polyamides are synthetic oligomers, which fold and bind to specific DNA sequences in a programmable manner. Internal side-by-side pairings of the aromatic amino acid residues 1-methyl-1H-pyrrole (Fy), 1-methyl-1H-inidazole [Im], and 3-hydroxy-1-methyl-1H-pyrrole (Fp) confer the ability to distinguish between all 4 Watson-Crick base pairs in the minor groove of B-form DNA. In a broad search to expand the heterocycle repertoire, we found that when 3-methylthiophene (Tn), which presents a S-atom to the minor groove, is paired with Py, it exhibits a modest 3-fold specificity for T-A > A-T, presumably by shape-selective recognition. In this study, we explore the scope and limitations of this lead by incorporating multiple Tn residues within a single heirpin polyamide. Hairpin polyamides containing >1 Tn/Py pair exhibit lowered affinities and specificities for their match sites. It appears that little deviation is permissible from the parent 5-membered ring 1-methyl-1H-pyrole-2-carboxamide scaffold for DNA recognition.

ACCESSION NUMBER: 2004:573249 HCAPLUS

DNA minor-groove recognition by 3-

TITLE:

AUTHOR (S):

141:407378

DNA minor-groove recognition by 3-methylthiophene/pyrrole pair
Doss, Raymond M.; Marques, Michael A.; Foister, Shane;
Dervan, Peter B.
Division of Chemistry and Chemical Engineering,
California Institute of Technology, Pasadena, CA,
91125, USA
Chemistry & Biodiversity (2004), 1{6}, 886-899
CODEN: CBMIAN; ISSN: 1612-1872
Verlag Helyetica Chimica Acta AG
Journal
English CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE: 791626-78-3P

PSI 522-78-3P
RL: ARG (Analytical reagent use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PPP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); PROC (Process); USES (Uses) (DNA minor-groove recognition by 3-methylthiophene/pyrrole pair) 791626-78-3 HCAPLUS (Margineering); PROC (dimethylamino)propyl] amino]-3-oxopropyl] amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-4-([(1-methyl-4-([(3-methyl-1-5-([(1-methyl-4-([(3-methyl-1-5-([(1-methyl-4-([(3-methyl-1-5-([(1-methyl-4-([(3-methyl-3-([3-methyl-3-([(3-methyl-3-([(3-methyl-3-([3-methyl-3-([(3-methyl-3-([(3-methyl-3-([3-methyl-3-([(3-methyl-3-([3-methyl-3-([(3-methyl-3-([3-methyl-

L8 ANSWER 2 OF 41 HCAPLUS COPYRIGHT 2005 ACS ON STN
ROBERT Neill III
PATENT ASSIGNEE(S): SNIKRLine Beecham Corporation, USA
PCT Int. Appl., 50 pp.
CODEN: PIXXD2 (Continued)

DOCUMENT TYPE: Patent LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA1	ENT	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D.	ATE	
						-									-		
WO	2004	0653	92		A1		2004	0805	,	WO 2	004-	EP65	0		2	0040	126
WO	2004	0653	92		C1		2004	1007									
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		BG,	BR,	BR,	BW,	BY,	BY,	BZ,	ΒZ,	CA,	CH,	CN,	CN,	co,	co,	CR,	CR,
		CU,	Cυ,	CZ,	CZ,	DE,	DE,	DK,	DK,	DM,	DZ,	EC,	EC,	EE,	EE,	EG,	ĖS,
		ES,	FI,	FI,	GB,	GD,	GE,	GE,	GH,	GM,	HR,	HR,	HU,	Hυ,	ID,	IL,	IN,
		IS,	J₽,	JP,	KE,	KE,	KG,	KG,	KP,	KP,	KP,	KR,	KR,	KZ,	ΚZ,	KZ,	LC,
		LK,	LR,	LS,	LS,	LT,	LU,	LV,	MA,	MD,	MD,	MG,	ΜK,	MN,	MW.	MX,	MX,
		MZ,	MZ,	NA,	NI												

A 20030124 A 20030415 A 20030702 PRIORITY APPLN. INFO.: GB 2003-1719 GB 2003-8706 GB 2003-15519

REFERENCE COUNT: THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-B

PAGE 2-A

791626-83-0P 791626-84-1P 791626-85-2P

RI: PRP (Properties): PUR (Purification or recovery); RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation): RACT (Reactant or reagent) (DNA minor-groove recognition by 3-methylthiophene/pyrrole pair) 791626-83-0 HCAPLUS

791626-83-0 HCAPLUS
2-Thiophenecarboxylic acid, 3-methyl-5-[[(1-methyl-4-nitro-1H-pyrrol-2-

ANSWER 3 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) y1)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

2-Thiophenecarboxylic acid, 5-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-3-methyl-, methyl ester (9CI) (CA INDEX NAME)

791626-85-2 HCAPLUS

2-Thiophenecarboxylic acid, 5-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-3-methyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION: (Continued)

PATENT NO. KIND DATE APPLICATION NO. DATE PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2004039799 A1 20040513 WO 2003-EP11805 20031024

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
GH, GM, HR, HU, DI, LI, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, MZ, NI, NO, NZ,
OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SI, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TH, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
BF, BJ, CF, CG, CI, CM, GA, GM, GG, GW, ML, MR, NE, SN, TD, TG
CA 2501739 AA 20040513 CA 2003-2501739 20031024

PI 1556377 A1 20050727 EP 2003-776869 20031024

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
PRIORITY APPLN. INFO:

MARPAT 140:4406731

TE, SI, LT, LV, FI, RO, MK, CY
PRIORITY APPLN. INFO::

OTHER SOURCE(S):

MARPAT 140:406731

IT 688324-04-1P 688924-05-2P 688924-06-3P
688324-10-1P 688924-10-5 88924-06-3P
688324-10-9P 688924-11-0P 688924-12-1P
688324-13-2P 6889224-11-0P 688924-12-1P
688324-13-2P 6889224-17-6P 688924-12-1P
688324-19-8P 689924-12-3P 689224-21-2P
688324-29-9P 689924-29-0P 689224-21-2P
688324-29-P 689924-25-6P 689224-27-8P
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689324-40-3P 689924-51-P
689324-50-7P 689924-51-P
689324-50-7P 689924-51-P
689324-56-3P 689924-55-P
689324-56-3P 689924-57-P
689324-56-3P 689924-57-P
689324-60-3P 689924-57-P
689324-71-P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES

(fungicide: preparation of N-(cyclopropylthienyl)carboxamides as fungicides) 688324-04-1 RCAPLUS 1H-Pyrrole-3-carboxamide, N-[3-(2-ethylcyclopropyl)-2-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 13 May 2004

A fungicidally active compound I, II, or III [wherein Het = (un) substituted 5- or 6-membered heterocyclic ring containing one to three O, N, and/or S atoms, provided that the ring is not 1,2,3-triazole: Rl and R2 = independently H, halo, or Mer. R3 = (un) substituted (cyclo)alkyl, alkenyl, alkynyl, Ph, heterocyclyl: R7 and R8 = independently H, halo, or (halo)alkyl) were prepared for use as active ingredients in agricultural or hotticultural compns. for controlling or preventing infestation of plants by phytopathogenic microorganisms, preferably fungi. For example, 3-difluoromethyl-1-methyl-1H-pyrazole-4-carboxylic acid was amidated with [2-(bicyclopropyl-2-yl) thiophen-3-yl] amine in the presence of TEA and N,N-bis(2-oxooxazolidinyl)phosphinic acid chloride in CH2C12 to give trans-IV [97s purity]. The latter showed excellent activity against Puccinia recondita on wheat (0-5% infestation) and showed good activity against Podosphaera leucotricha on apple, Venturia inaequalis on apple, Erysiphe graminis on barley, Pyrenophora teres on barley, Alternaria solani on tomato, and Uncinula necator on grape (<20% infestation for each).

each).
ACCESSION NUMBER:
DOCUMENT NUMBER:
TITLE: 2004:390242 HCAPLUS 140:406731

Preparation of N-(cyclopropylthienyl)carboxamides as

Tungicides

Ehrenfreund, Josef: Tobler, Hans, Walter, Harald
Syngenta Participations Ag, Switz.

PCT Int. Appl., 43 pp.

CODEN: PIXXD2 INVENTOR(S): PATENT ASSIGNEE(S):

ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688324-05-2 HCAPLUS
1H-Pyrrole-3-carboxamide, N-[3-(2-ethylcyclopropyl)-2-thienyl]-1(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688324-06-3 HCAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[3-(2-propylcyclopropyl)-2-thienyl]-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

688324-07-4 HCAPLUS IH-Fyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[3-(2-propylcyclopropyl)-2-thienyl]- (9CI) (CA INDEX NAME)

688324-08-5 HCAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-n-[3-[2-(1-methylethyl)cyclopropyl]-2-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-09-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[3-[2-(1-methylethyl)cyclopropyl]-2-thienyl]- (9CI) (CA INDEX NAME)

RN 688324-10-9 HCAPLUS
CN 1H-Pyrclol-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-[3-[2-(1-methylethyl)-cylopropyl]-2-thienyl]- (9CI) (CA IMDEX NAME)

RN 688324-11-0 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-(3-[2-(1-methylethyll-yelopropyl]-2-thlenyl]- (9Cl) (CA INDEX NAME)

RN 688324-12-1 HCAPLUS

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-16-5 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-butylcyclopropyl)-2-thienyl]-1-methyl-4(trifluoromethyl)- (SCI) (CA INDEX NAME)

RN 688324-17-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{3-(2-butylcyclopropyl)-2-thienyl}-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-18-7 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-butylcyclopropyl)-2-thienyl]-2-fluoro1,4-dimethyl- (9C1) (CA INDEX NAME)

RN 688324-19-8 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-butylcyclopropyl)-2-thienyl}-2-chloro1,4-dimethyl- (9C1) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1-ethyl-4-methyl-N-[3-[2-{1-methylethyl}cyclopropyl]-2-thienyl]- (9CI) (CA INDEX NAME)

RN 688324-13-2 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-{3-{2-{1-methylethyl}cyclopropyl}-2-thienyl}- (9CI) (CA INDEX NAME)

RN 688324-14-3 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-ethyl-2-fluoro-4-methyl-N-{3-{2-(1-methylethyl)cyclopropyl}-2-thienyl}- (9CI) (CA INDEX NAME)

RN 688324-15-4 HCAPLUS
CN H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-2-fluoro-1-methyl-N-[3-[2-(1-methyl-thyl)cyclopropyl]-2-thienyl]- (SCI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-20-1 HCAPLUS
CN H-Fyrrole-3-carboxamide, 1-methyl-N-[3-[2-(2-methylpropyl)cyclopropyl]-2-thienyi]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-21-2 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-{3-[2-(2-methylpropyl)cyclopropyl]-2-thienyl]- (9CI) (CA INDEX NAME)

RN 688324-22-3 HCAPLUS CM 1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-(3-[2-(2-methylpropyl)cyclopropyl)-2-thienyl)- (9CI) (CA INDEX NAME)

RN 688324-23-4 HCAPLUS

IN-Pyrrole-3-carboxamide, 1-(methoxymethyl)-N-{3-[2-(2-methylpropyl)cyclopropyl)-2-thienyl]-4-(trifluoromethyl)- (9C1) (CA INDEX NAME)

ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688324-24-5 HCAPLUS
1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-[3-[2-(2-methylpropyl)cyclopropyl]-2-thienyl]- (9CI) (CA INDEX NAME)

688324-25-6 HCAPLUS
1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[3-[2-{2-methylpropyl})cyclopropyl]-2-thienyl)- (9CI) (CA INDEX NAME)

688324-26-7 HCAPLUS
1H-Pyroole-3-carboxamide, N-(3-(2-(1,1-dimethylethyl)cyclopropyl]-2-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688324-31-4 HCAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[3-{2-pentylcyclopropyl}-2-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688324-32-5 HCAPLUS 1H-Pytrole-3-carboxamide, 1-methyl-N-(3-[2-(3-methylbutyl)cyclopropyl]-2-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688324-33-6 HCAPLUS 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[3-[2-(3-methylbutyl)cyclopropyl]-2-thienyl]- (9CI) (CA INDEX NAME)

688324-34-7 HCAPLUS 1H-Pyrrole-3-carboxemide, N-[3-(2-hexylcyclopropyl)-2-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 688324-27-8 HCAPLUS | H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-N-[3-[2-(1,1-dimethylethyl)cyclopropyl]-2-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

688324-28-9 HCAPLUS
1H-Pyrrole-3-carboxamide, N-[3-[2-[1,1-dimethylethyl]cyclopropyl]-2-thienyl]-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

688324-29-0 HCAPLUS

IH-Pyrrole-3-carboxamide, 2-chloro-N-[3-[2-[1,1-dimethylethyl)cyclopropyl]-2-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

688324-30-3 HCAPLUS
1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[3-[2-(1,1-dimethylethyl)cyclopropyl]-2-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688324-35-8 HCAPLUS
1H-Pyrrole-3-carboxamide, N-(3-[1,1'-bicyclopropyl]-2-yl-2-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688324-36-9 HCAPLUS
1H-Pyrrole-3-carboxamide, N-(3-{1,1'-bicyclopropyl}-2-yl-2-thienyl)-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

688324-37-0 HCAPLUS 1H-Pyrrole-3-carboxamide, N-(3-(1,1'-bicyclopropyl)-2-yl-2-thienyl)-2-fluoro-1,4-dimethyl- (9C1) (CA INDEX NAME)

688324-38-1 HCAPLUS
1H-Pyrrole-3-carboxamide, N-(3-(1,1'-bicyclopropyl)-2-yl-2-thienyl)-2-chloro-1,4-dimethyl- (9CI) (CA INDEX NAME)

LB ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

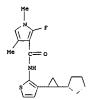
RN 688324-39-2 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cyclobutylcyclopropyl)-2-thienyl]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-40-5 HCAPLUS CN H-Pyrrole3-carboxsmide, N-[3-(2-cyclobutylcyclopropyl)-2-thienyl]-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-41-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cyclopentylcyclopropyl)-2-thienyl]-1methyl-4-(crifluoromethyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) cyclopentylcyclopropyl)-2-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-45-0 HCAPLUS
CN HH-Fyrrole-3-carboxamide, N-[3-(2-cyclopentylcyclopropyl)-2-thienyl]-2-fluoro-1,4-dimethyl- (SCI) (CA INDEX NAME)



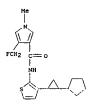
RN 688324-47-2 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-N-[3-(2-cyclopentylcyclopropyl)-2-thienyl]-1, 4-dimethyl- (9CI) (CA INDEX NAME)

RN 688324-48-3 HCAPLUS
CN 1H-Pyrclo1-3-carboxamide, N-[3-(2-cyclohexylcyclopropyl)-2-thienyl]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-42-7 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cyclopentylcyclopropyl)-2-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-43-8 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cyclopentylcyclopropyl)-2-thienyl]-4(fluormethyl)-1-methyl- (9CI) (CA INDEX NAME)



RN 688324-44-9 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[3-(2-

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-49-4 HCAPLUS CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cyclohexylcyclopropyl)-2-thienyl]-4-(difluoromethyl)-1-methyl- (9C1) (CA INDEX NAME)

RN 688324-50-7 HCAPLUS
CN H-Pyrrole-3-carboxamide, N-[3-(2-cyclohexylcyclopropyl)-2-thienyl]-4(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-51-8 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[3-{2cyclohexylcyclopropyl]-2-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-52-9 HCAPLUS CN H-Pyrrole-3-carboxamide, N-[3-(3-cyclohexyl-2,2-difluorocyclopropyl)-2thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

LB ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me N CF3 F

RN 688324-53-0 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cyclohexylcyclopropyl)-2-thienyl]-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688324-54-1 HCAPLUS CN H-Pyrclo-3-carboxamide, 2-chloro-N-(3-(2-cyclohexylcyclopropyl)-2thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

Me C1 S

RN 688324-55-2 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cycloheptylcyclopropyl)-2-thienyl]-1methyl-4-(trifluoromethyl)- (9C1) (CA INDEX NAME)

Me N C-NH S

RN 688324-56-3 HCAPLUS

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-60-9 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cycloheptylcyclopropyl)-2-thienyl]-2-fluoro-1,4-dimethyl- (9C1) (CA INDEX NAME)

RN 688324-61-0 HCAPLUS
CN 1H-Pyrclol-3-carboxamide, 2-chloro-N-[3-(2-cycloheptylcyclopropyl)-2-thlenyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

Me O C S S S Me C1

RN 688324-62-1 HCAPLUS
CN 1H-Fyrrole-3-carboxamide, N-{3-(2-cyclooctylcyclopropyl)-2-thienyl}-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me N C-NH S

RN 688324-63-2 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-[2-cyclooctylcyclopropyl]-2-thienyl]-4(diffluoromethyl)-1-methyl- [9CI] (CA INDEX NAME)

Page 1530/08/2005

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cycloheptylcyclopropyl)-2-thienyl]-1ethyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

CF3

RN 688324-57-4 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cycloheptylcyclopropyl)-2-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

Me O C-NH S

RN 688324-58-5 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cycloheptylcyclopropyl)-2-thienyl]-4(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

0 || C-NH-|| S

RN 688324-59-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[3-[2-cycloheptylcyclopropyl)-2-thienyl]-2-fluoro-1-methyl- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me N S CHF2

RN 688324-64-3 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[3-(2-phenylcyclopropyl)-2-thienyl]-4(trifluoromethyl)- (9C1) (CA INDEX NAME)

Me N CF3

RN 688324-65-4 HCAPLUS CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-{3-(2-phenylcyclopropyl)-2-thienyl]- (9CI) (CA INDEX NAME)

Me N CHF2

RN 688324-66-5 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-(3-(2-phenylcyclopropyl)-2-thienyl]- (SCI) (CA INDEX NAME)

Me N C-NH S

RN 688324-67-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-[3-(2-phenylcyclopropyl)-2-thienyl]- [9C1) (CA INDEX NAME)

ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688324-68-7 HCAPLUS
1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-{3-(2-phenylcyclopropyl)-2-thienyl}- (9CI) (CA INDEX NAME)

688324-69-8 HCAPLUS
1H-Pyrrole-3-carboxamide, N-[3-[2-(4-fluorophenyl)cyclopropyl]-2-thienyl]1-methyl-4-(trifluoromethyl)- [9CI] (CA INDEX NAME)

688324-70-1 HCAPLUS
1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-N-[3-[2-(4-fluorophenyl)cyclopropyl]-2-thienyl)-1-methyl- (9CI) (CA INDEX NAME)

688324-71-2 HCAPLUS

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

688324-75-6 HCAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[3-[2-(2-thienyl)cyclopropyl]-2-thienyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688324-76-7 HCAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[3-[2-(3-thienyl)cyclopropyl]-2-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688324-77-8 HCAPLUS
1H-Pyrrole-3-carboxamide, N-[3-[2-(2-furanyl)cyclopropyl]-2-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688324-78-9 HCAPLUS

Page 1630/08/2005

ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STM (Continued) 1H-Pyrrole-3-cerboxamide, N-(3-12-(4-chlorophenyl)cyclopropyl)-2-thienyl)-1-methyl-4-(trifluoromethyl)-(9C1) (CA INDEX NAME)

688324-72-3 HCAPLUS
1H-Pyrrole-3-carboxamide, N-[3-[2-[4-chlorophenyl]cyclopropyl]-2-thienyl]-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

688324-73-4 HCAPLUS
1H-Pyrrole-3-carboxamide, N-[3-[2-(4-bromophenyl)cyclopropyl]-2-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688324-74-5 HCAPLUS
1H-Pyrrole-3-carboxamide, N-(3-(2-(4-bromophenyl)cyclopropyl]-2-thienyl]-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 1H-Pytrole-3-carboxamide, N-[3-[2-(3-furany1)eyclopropy1]-2-thieny1]-1-methy1-4-(trifluoromethy1)- 9(5)1 (CA INDEX MAME)

688324-79-0 HCAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[3-(1'-methyl[1,1'-bicyclopropyl]-2-yl)-2-thienyl]-4-(CA IMDEX NAME)

688324-80-3 HCAPLUS
1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[3-(1'-methyl[1,1'-bicyclopropyl]-2-yl)-2-thienyl]- (9CI) (CA INDEX NAME)

688324-81-4 HCAPLUS
HH-Pyrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-[3-(1'-methyl[1,1'-blcyclopropyl]-2-yl)-2-thienyl]- (SCI) (CA INDEX NAME)

ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688324-82-5 HCAPLUS |H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-(3-(1'-methyl(1,1'-bicyclopropyl]-2-yl)-2-thienyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 683815-41-0 HCAPLUS HH-Pyrrole-2-carboxamide, 4-(acetylamino)-N-[4-[[[5-([[3-(dimethylamino)propyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-5-methyl-2-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

IT 683815-68-1P

683815-68-1P
RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, antimicrobial and antifungal activities of heterocyclic amino acid trimers as distamycin analogs with enhanced lipophilicity)
683815-68-1 RCAPUUS
HF-Pyrrole-2-carboxamide, N-[4-[[[5-[[3-(dimethylamino)propyl]amino]carbo nyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-5-methyl-2-thienyl]-1-methyl-4-nitro- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 05 Mar 2004 Forty-eight heterocyclic amino acid trimers, analogs of distamycin, with a number of features that enhance lipophilicity are described. They contain alkyl or cycloalkyl groups larger than methyl; some are N-terminated by acetamide or methoxybenzamide and are C-terminated by dimethylaminopropyl or aliphatic heterocyclic aminopropyl substituents. The ability of these compds. to bind principally to AT tracts of DNA has been evaluated using capillary zone electrophoresis. Significant antimicrobial activity against key organisms such as MRSA and Candida albicans is shown by several compds., especially those containing a thiazole. Moreover, these ds.

Compds.

Accession Number:
ACCESSION NUMBER:
DOCUMENT NUMBER:
100:375474

AUTHOR(S):
AUTHOR(S):
CORPORATE SOURCE:
Source:
Classow, Gl 1XL, UK
SOURCE:
Journal of Medicinal Chemistry and Department of Pharmaceutical Sciences, University of Strathclyde, Glassow, Gl 1XL, UK
SOURCE:
DOUBLISHER:
American Chemical Society
DOCUMENT TYPE:
Journal LANGUAGE:
Book: English

DOCUMENT TYPE: LANGUAGE:

MENT TYPE: Journal
UNGE: English
683815-40-9P 683815-41-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(preparation, antimicrobial and antifungal activities of heterocyclic amino
acid trimers as distamycin analogs with enhanced lipophilicity)
683815-40-9 HCAPLUS
HI-Pyrrole-2-carboxamide, N-(4-[[[5-([[3-(dimethylamino)propyl]amino]carbo
nyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-5-methyl-2-thienyl]-4(formylamino)-1-methyl- (9CI) (CA INDEX NAME)

LB ANSWER 6 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 02 Sep 2003

AB The eight novel polyamides: PyPyPyBDp, ImPyPpyBDp,
ImImPyBDp, PyImImBDp, ImImImBDp, PyPyImBDp,
ImiPyImpDp, and PyImPyBDp (Py = N-methylpyrrole, Im =
N-methylimidazole, β = β-alanine, Dp = N.Ndimethylpropyldiamine) were synthesized by the dicyclohexylcarbodimide/1hydroxybenzotriazole (DCC/HOB1) coupling reaction. This paper describes
the mass spectral fragmentation mechanisms of these eight polyamides,
investigated by electrospray ionization with tandem mass spectrometry
(ESI-MS/MS). 2003:684284 HCAPLUS
DCCUMENT NUMBER:
2003:684284 HCAPLUS
TITLE:
Fragmentation mechanisms of polyamides containing
N-methylpyrole and N-methylpyrids202 by alexance.

Fragmentation mechanisms of polyamides containing N-methylpyrrole and N-methylimidezole by electrospray ionization tandem mass spectrometry Yuen, Gu; Tang, Feili; Zhu, Chang Jin; Liu, Yan; Zhao,

AUTHOR (5):

Yu Fen
Department of Chemical Biology, The Key Laboratory of
Bioorganic Chemistry and Molecular Engineering,
Ministry of Education, College of Chemistry, Peking
University, Beijing, 100871, Peop. Rep. China
Rapid Communications in Mass Spectrometry (2003),
17(17), 2015-2018
CODEN: RCMSPE: ISSN: 0951-4198
John Wiley & Sons Ltd.
Journal CORPORATE SOURCE:

SOURCE:

PUBLISHER: Journal

DOCUMENT TYPE: LANGUAGE:

MENT TYPE: Journal
UAGE: English
648928-24-9P 648928-25-0P 648928-29-4P
RL: CPS (Chemical process): PEP (Physical, engineering or chemical
process): SPN (Synthetic preparation): PREP (Preparation): PROC (Process)
(fragmentation mechanisms of polyamides contesining methylpyrrole and
methylimidazole by electrospray ionization tandem mass spectrometry)
648928-24-9 HCAPLUS
IH-Pyrrole-2-carboxamide. N-[5-[[[3-[[3-(dimethylamino)propyl]amino]a-3oxopropyl]amino[actboxyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-5-[([1-methylIH-pyrrol-2-yl)carbonyl]amino]- (9CI) (CA INDEX NAME)

PAGE 1-B



648928-25-0 HCAPLUS

1H-Imidazole-2-carboxamide, N-[5-[[[5-[[3-[{3-(dimethylamino]propyl]amino]-3-oxopropyl]amino]carbonyl]-1-methyl-1Hpyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl- (9CI) (CA
INDEX NAME)

L8 ANSWER 6 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-B

648928-29-4 HCAPLUS
1H-Imidazole-2-carboxamide, N-[3-[[3-(dimethylamino)propyl]amino]-3oxopropyl]-1-methyl-5-[[[1-methyl-18-pyrrol-2yl)carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

PAGE 1-B

REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)
9J, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU 200108187 A5 20020313 AU 2001-80187 20010827
PRIORITY APPLN. INFO.: JP 2000-257451 A 20000828

OTHER SOURCE(S): MARPAT 136:232201

IT 403617-43-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Uses)
(preparation of cyclic amine derivs. as CCR3 antagoniata)
(30517-43-6 MCAPLUS
1,2-Pyrrolidinedicarboxamide, NZ-(3-cyano-2-thienyl)-Nl-((3-exo)-8-{(6-fluoro-2-naphthalenyl)methyl]-8-azabicyclo[3.2.1]oct-3-yl}-, (2S)- (9CI)
(CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Page 1830/08/2005

ANSWER 7 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 08 Mar 2002

AB The title compds. I [ring A = {un}substituted heterocyclic ring, etc.; X = bond, O, CO, etc.; ring B = Q1, etc.; ring V3 = hydrocarbon ring, etc.; W = CH, N; Y = CO, etc.; R21, R22 = H, halo, etc.; T1 = {CH2}n; n = 0 - 2; ring D = {un}substituted aryl, etc.} are prepared In an in vitro test (for CCR3 antagonism) using cells, compds. of this invention showed IC50 values of 0.001 kM to 0.45 kM.

ACCESSION NUMBER: 2002:171853 HCAPLUS
DOCUMENT NUMBER: 136:232201
TITLE: Preparation of cyclic amine derivatives as CCR3 antagonists
Morihira, Koichiro: Inami, Hiroshi; Kubota, Hirokazu; Yokoyama, Kazuhiro: Morokata, Tatsuaki; Takeuchi, Makoto: Takahashi, Toshiya: Kaneko, Masayuki; Imaoka, Takayuki; Torii, Yuichi; Iura, Yosuke
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan; Toray Industries, Inc.
PCT Int. Appl., 92 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILIY ACC. NUM. COUNT: 1
PATENT INFORMATION:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	ENT :	NO.			KIN	Ď	DATE			APPL	CAT	ION	NO.		Di	ATE	
						-											
WO	2002	0183	35		A1		2002	0307	1	WO 2	001-	JP73.	21		2	0010	827
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GÉ,	GH,
		GM,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MΑ,	MD,	MG,	MK,	MN,	MW,	ΜX,	MZ,	NO,	NZ,	PH,	PL,
		PT,	RO,	RU,	SD,	SÈ,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,
		US,	UZ,	VN,	YU,	ZA,	ZW.	AM,	AZ,	BY,	KG,	ΚZ,	MD,	RU,	ΤJ,	TM	
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,
		DE.	DK	PC	FT	FD	CB	GB	TE	TT	1.11	MC	NT.	DT	SE:	TR	BF.

L8 ANSWER 7 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ANSWER 8 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 28 Dec 2001

AB The title compds. [I: R1, R2 = H, halo, ary1, etc.: or R1 and R2 taken together form (CH2)m(NR4)n(CH2)p (wherein m, p = 1-3: n = 0-1; m + n + p = 3-5; R4 = H, alky1); R3 = alky1, alkeny1, ary1, etc.], useful in the treatment of diseases caused by and/or associated with an altered protein kinase activity such as cancer, cell proliferative disorders, Alzheimer's disease, viral infections, auto-inmune diseases and neurodegenerative disorders (no data given), were prepared Thus, amidation of 2-aminon-3-carbomy1-4, 5, 6, 7-tetrahydrobenzo|0|thiophene with phenylacetic acid afforded I [R1R2 = (CH2)4; R3 = CH2Ph].

ACCESSION NUMBER: 2001:935593 HCAPLUS

DOCUMENT NUMBER: 136:69729

INVENTOR(S): Preparation of thiophene-3-carboxamides as kinase inhibitors

INVENTOR(S): Preparation of thiophene-3-carboxamides as kinase inhibitors

INVENTOR(S): Parent Assignee (S): Pharmacia & Upjohn S.p.A., Italy

POCUMENT TYPE: Parent Appl., 85 pp.

COODEN: PIXXD2

DOCUMENT TYPE: Parent

English

LANGUAGE: Patent
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PA1	ENT	NO.					DATE								D	ATE	
						-									-		
WO	2001	0982	90		A2		2001	1227	1	WO 2	001-1	EP67	63		2	0010	614
WO	2001	0982	90		A3		2002	0516									
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ВŻ,	CA,	CH,	CN,
		co.	CR,	CU,	CZ,	DE.	DK,	DM,	DZ,	EC,	EE,	ES,	FI.	GB,	GD.	GE,	GH,
		GM,	HR.	HU,	ID,	IL,	IN,	IS,	JP.	KE,	KG.	KP.	KR,	KZ,	LC.	LK,	LR,
		LS.	LT.	LU.	LV,	MA.	MD,	MG,	MK.	MN,	MW.	MX,	MZ,	NO,	NZ.	PL,	PT.
		RO,	RU,	SD,	SE,	SG.	SI,	SK,	SL,	TJ,	TM.	TR,	TT.	TZ,	UA.	UG,	US,
		UZ.	VN.	YU,	ZA.	ZW.	AM,	AZ.	BY,	KG,	KZ.	MD,	RU.	TJ.	TM		
	RW:	GH.	GM.	KE,	LS.	MW.	MZ.	SD,	SL.	SZ.	TZ.	UG.	ZW.	AT.	BE,	CH,	CY,
		DE.	DK.	ES,	FI.	FR.	GB,	GR.	IE.	IT.	LU.	MC.	NL.	PT.	SE,	TR,	BF,
		BJ,	CF.	CG,	CI.	CM.	GA.	GN,	GW,	ML.	MR.	NE.	SN,	TD.	TG		
US	6414	013			В1		2002	0702		US 2	000-	5965	50		2	0000	619
CA	2414	085			AA		2001	1227		CA 2	001-	2414	085		2	0010	614
ΑU	2001	0857	45		A5		2002	0102		AU 2	001-	8574	5		2	0010	614
ΕP	1294	707			A2		2003	0326		EP 2	001-	9649	83		2	0010	614
	R:	AT,	ΒE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,

ANSWER 8 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

383380-90-3 HCAPLUS 2-Pyrrolidinecarboxamide, l-acetyl-N-[3-(aminocarbonyl)-5-(1-phenylethyl)-2-thienyl]-4-hydroxy- (9CI) (CA INDEX NAME)

383381-04-2 HCAPLUS
1H-Indole-2-carboxamide, N-[3-(aminocarbonyl)-5-(1-phenylethyl)-2-thienyl]1-methyl- (9CI) (CA INDEX NAME)

383381-05-3 HCAPLUS

HH-Indole-3-carboxamide, N-{3-(aminocarbonyl)-5-(1-phenylethyl)-2-thienyl}-1-methyl- (9CI) (CA INDEX NAME)

Page 1930/08/2005

L8 ANSWER 8 OF 41 HCAPLUS COPYRIGHT 2005 ACS ON STN
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2004501146 T2 20040115 JP 2002-504246
PRIORITY APPLN. INFO.: US 2000-596550
WO 2001-EP6763 (Continued) 20010614 A 20000619 W 20010614 OTHER SOURCE(S): MARPAT 136:69729
IT 383379-42-09 383379-77-99 383380-21-09 383380-99-39 383381-04-29 383380-21-09 RL: PAC (Pharmacological activity): SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation of thiophene-3-carboxamides as kinase inhibitors)
383379-42-8 KCAPLUS
HT-Pyrrole-2-carboxamide, N-[3-(aminocarbonyl)-4,5,6,7tetrahydrobenzo[b]thien-2-yl]-1-methyl- (9CI) (CA INDEX NAME)

383379-77-9 HCAPLUS 2-Pyrrolidi-

2-Pyrrolidinecarboxamide, N-[3-(aminocarbonyl)-5-(1-methylethyl)-2-thienyl]-1-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

383380-21-0 HCAPLUS 2-Pyrrolidinecarboxamide, 1-acety1-N-[3-(aminocarbony1)-5-pheny1-2-thieny1]- (9CI) (CA INDEX NAME)

(Continued) L8 ANSWER 8 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ANSWER 9 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: $26\ \text{Sep}\ 2000$

AB N-linked five-membered heteroaryls were obtained by conversion of 2-carboxy-heteroarenes I (Y = OH, R = H, Me, SiMe3, X = S, Se, O) into N-(2-heteroaryl)-1-methylpyrrole-2-carboxamides II. The procedure is based on a simple thermal rearrangement of thiophene or selenophene carbonyl arides I (Y = N3) in neat 1-methylpyrrole at 90°.

ACCESSION NUMBER: 2000:673727 HCAPLUS

DOCUMENT NUMBER: 134:10944

A convenient and efficient conversion of 2-carboxyheteroarenes into and N-(2-thienyl and 2-selenophenyl) 1-methylpyrrole-2-carboxamides

Danielli, Filippor Zanirato, Paolo

Dip. di Chim. Organica, 'A. Mangini', Univ. di

Bologna, Bologna, 40136, Italy

ARKIVOC (online computer file) (2000), 1(1), '67-72

CODEN: AKVCFI

URL: http://www.arkat.org/arkat/journal/Issuel/ARK0000

09/ms9.pdf

PUBLISHER: ARKAT Foundation

DOCUMENT TYPE: Journal; (online computer file)

English

CTHER BOURCE(S): CASREACT 134:100944

CASREACT 134:100944

319447-91-1P 319447-95-5P 319447-97-7P 319447-99-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 319447-91-1. MCAPUUS 1+Pyrrole-2-carboxamide 1-methyl-N-2-thienyl- (9C

1-methyl-N-2-thienyl- (9CI) (CA INDEX NAME)

ANSWER 10 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 15 Sep 2000
A new aromatic pair, 2-hydroxy-6-methoxybenzamide/1-methylpyrrole at the terminal position of hairpin polyamides has been designed for distinguishing T-A from A-T base pairs and both from G-C/C-G in the minor groove of DNA. Four eight-ring hairpin polyamides with benzamide (Bz), 2-hydroxybenzamide (Hb-1), 2-hydroxy-6-methylbynzamide (Hb-2), and 2-hydroxy-6-methylbynzamide (Hb-3) at the N-terminal position were synthesized. The equilibrium ciation

association

consts. (Ka) were determined at four DNA sites which differ at a single commo consts. (Ka) were determined at four DNA sites which differ at a single commo position, 5'-TNTACA-3' (N = T, A, G, C). Quant. DNase I footprint titration expts. reveal that (Rb-3)PyPyPy-(R)H2Ny-ImPyPyPy-B-Dp (4) bound the sequences 5'-TTTACA-3' and 5'-TTTACA-3' with high affinity. Ka = 2.6 + 1010 M-1 and Ka = 8.4 + 109 M-1, resp., a 3-fold specificity for T vs. A was found. Importantly, the sequences 5'-TCTACA-3' and 5'-TCTACA-3' are bound with 50 and 200 times lower affinity, revealing an overall specificity of Hb-3/Py of T > A > G > C. These results are supported to the sequences targetable by hairpin polyamides.

ACCESSION NUMBER: 2000:644918 HCAPLUS
DOCUMENT NUMBER: 134:26617

DOCUMENT NUMBER: 134:26617

134:26617

Hydroxybenzamide/Pyrrole Pair Distinguishes T-A
from A-T Base Pairs in the Minor Groove of DNA
Ellervik, Ulf: Wang, Clay C. C.; Dervan, Peter B.
Division of Chemistry and Chemical Engineering,
California Institute of Technology, Pasadena, CA,
91125, USA
Journal of the American Chemical Society (2000),
122(39), 9354-9360
CODEN: JACSAT; ISSN: 0002-7863
American Chemical Society
Journal
English AUTHOR(S): CORPORATE SOURCE:

SOURCE:

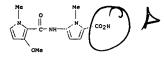
PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

312299-02-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

RL: RCT (Reactant): SPN (Synthetic preparation): rRET (Freparation): rock (Reactant or reagent)
(polyamides containing hydroxybenzamide/pyrrole pair distinguish T-A from A-T base pairs in minor groove of DNA)
312299-02-8 HCAPLUS
H-Pyrrole-2-carboxylic acid, 5-[[(3-methoxy-1-methyl-1H-pyrrol-2-yl)carbonyl]amino]-1-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 9 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 1H-Pyrrole-2-carboxamide, N-2-furanyl-1-methyl- (9CI) (CA INDEX NAME)

319447-97-7 HCAPLUS 1H-Pyrrole-2-carboxamide, 1-methyl-N-(5-methyl-2-thienyl)- (9CI) (CA INDEX NAME

319447-99-9 HCAPLUS

xamide, 1-methyl-N-[5-(trimethylsilyl)-2-thlenyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 13 Jul 2000

AB Head-to-head linked dimers of heterocyclic amino acids were prepared to investigate their affinity and selectivity in binding to the minor groove of DNA. The selection of targets for synthesis was led by computer based design. Several novel dicarboxylic acid linkers including indoles, phenanthrenes, a fluorenone, and a bisbenzothiophene were included. Anal. of binding to DNB by footprinting showed high affinity for compds. derived from 2,7-dihydrophenanthrenedicarboxylic acid and a predominate selectivity for AT rich regions containing at least four AT pairs but with the ability to span up to two CG base pairs.

ACCESSION NUMBER: 2000:471732 HCAPLUS

DOCUMENT NUMBER: 133:281718

133:281718

TITLE:

AUTHOR (S):

133:281718
The synthesis of some head to head linked DNA minor groove binders
Khalaf, A. I.; Pitt, A. R.; Scobie, M.; Suckling, C. J.; Urwin, J.; Waigh, R. D.; Fishleigh, R. V.; Young, S. C.; Wylie, W. A.
Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow, Gl IXL, UK
Tetrahedron (2000), 56(29), 522-5239
CODEN: TETRAB; ISSN: 0040-4020
Elsevier Science Ltd.
Journal
English CORPORATE SOURCE:

SOURCE:

PUBLISHER

DOCUMENT TYPE: LANGUAGE:

English CASREACT 133:281718 OTHER SOURCE(S):

299974-91-7P

Z99974-91-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of head-to-head linked heterocyclic amino acid dimers with binding affinity to minor groove of DNA)
299974-91-7 HCAPLUS
HH-Pyrrole-2-carboxamide, N-[5-[[(3-(dimethylamino)propyl]amino]carbonyl]-2-thienyl]-1-methyl-4-nitro- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 12 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 12 May 2000

AB A process of synthesizing a bicyclo compound (I) is described. Proline (II) is reacted with diphenylphosphinic chloride to activate the carboxylic acid group, and then reacted with methanesulfonyl chloride to produce ester (III) which is then reacted with a group II metal sulfide source in water to produce I.

CCCESSION NUMBER: 2000:307143 HCAPLUS

DOCUME:

2000:307143 HCAPLUS
132:321855
Process for synthesizing carbapenem side chain intermediates
Brands, Karel M. J.; Williams, John M.; Dolling, Ulf
H.; Jobson, Ronald B.; Davies, Antony J.; Cottrell,
Ian F.; Cameron, Mark; Ashwood, Michael S.
Merck and Co., Inc., USA
U.S., 13 pp., Division of U.S. Ser. No. 106,297.
CODEN: USXXAM
Patent
English INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6060607	A	20000509	US 1999~334398	19990616
US 6063931	А	20000516	US 1998-106297	19980629
PRIORITY APPLN. INFO.:			US 1998~106297 A3	19980629
			US 1997-52032P P	19970709
OTHER SOURCE(S):	CASRE	ACT 132:3218	55; MARPAT 132:321855	

266337-28-4P

266337-28-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for synthesizing carbapenem side chain intermediates)
266337-28-4 HCAPLUS
1-Pyrrolidinecarboxylic acid, 2-{[(5-carboxy-2-thienyl)amino]carbonyl}-4-hydroxy-, 1-(1,1-dimethylethyl) ester, (2S,4S)- (9CI) (CA INDEX NAME)

ANSWER 13 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 07 Apr 2000 A synthetic combinatorial library of 10,000 components mostly containing atic

A synthetic Combinatorial Indiary of 10,000 Components aboutly Containing after amino acids was screened for inhibition of DNase I cleavage at two ARE sequences. Ten amino acid building blocks were used to generate the library in which the N and C terminal residues were fixed and the four central positions of the peptide ligands were varied. The DNase I footprinting assay led, after deconvolution through sublibrary synthesis, to the identification of CGL-6382 as an ARE-selective minor groove binder containing a N-terminal nicotinic acid motif adjacent to a N-methylimidazole unit and three N-methylpyrole units coupled to a C-terminal argininamide residue. The optimized ligand CGL-6382 was found to recognize a 5°-GC(AY) (AY) motif within the two cloned androgen receptors responsive elements. The discovery of CGL-6382 as an ARE-selective ligand augurs well for the use of the DNase I footprinting methodol. to identify sequence-specific DNa recognition ligands from large mixts. of small mols. (c) 2000 Academic Press.

SSION NUMBER: 2000:224933 HCAPLUS

LEMT NUMBER: 133:66541

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

AUTHOR (S):

CORPORATE SOURCE:

2000:224933 HCAPLUS
133:68541
An ARE-selective DNA minor groove binder from a combinatorial approach Hamy, Francois; Albrecht, Genevieve; Florsheimer, Andreas; Bailly, Christian Department of Oncology, Novartis Pharma Research, Basel, CH-4002, Switz.
Blochemical and Blophysical Research Communications (2000), 270(2), 393-399
CODEN: BBRCA9; ISSN: 0006-291X Academic Press
Journal SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

English

278788-95-7P

RE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(an ARE-selective DNA minor groove binder from a combinatorial

approach) 278788-95-7 HCAPLUS

2/8788-95-7 HCAPLUS
3-Pyridinecarboxamide, N-[2-[[[5-[[[5-[[[5-[[[5-[[3-[diaminoiminomethyl]amino]propyl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]- (9CI) (CA INDEX NAME)

ANSWER 12 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN lute stereochemistry. (Continued)

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 13 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 01 Dec 1999
BT the synthesis, biol. activity, and DNA-binding properties of a series of
four pyrrolo[2,1-c][1,4]benzodiazepine (PBD) hybrids containing polypyrrole
side chains are described and structure-activity relationships examined To
investigate sequence selectivity and stability of drug/DNA complexes,
DNase I footprinting and arrested polymerase chain reaction (PCR) were
performed on human c-myc oncogene, estrogen receptor gene, and human
immunodeficiency virus type I long terminal repeat (HIV-I LTR) gene
sequences. The antiproliferative activity of the hybrids was tested in
vitro on human myeloid leukemia K562 and T-lymphoid Jurkat cell lines and
compared to antiproliferative effects of the natural product distamycin A
1, its tetrapyrrole homolog, DC 81, and a PBD ester. The new hybrids
exhibit different DNA-binding activity with respect to both distamycin A 1
and the parent PBD. In addition, a direct relationship was found between the
number of pyrrole rings present in the hybrids and the stability of drug/DNA
complexes. With respect to antiproliferative effects, i.e., the hybrid with
pyrroles is more active than the other ones both against K562 and Jurkat
cell lines.

ACCESSION NUMBER:

1999:758546 HCAPLUS

DOCUMENT NUMBER:

1999:758546 HCAPLUS

Synthesis, in Vitro Antiproliferative Activity, and
DNA-Binding Properties of Hybrid Molecules Containing
Pyrrolo[2,1-c](1,4]themodalaraenine and

increase of in vitro antiproliferative effects, 1.e., the hybrid with 4 pyrroles is more active than the other ones both against K562 and Jurkat cell lines.

ACCESSION NUMBER: 1999:758546 HCAPLUS
DOCUMENT NUMBER: 132:137361

TITLE: Synthesis, in Vitro Antiproliferative Activity, and DNA-Binding Properties of Hybrid Molecules Containing Pyrrolo[2,1-c][1,4]benzodiazepine and Minor-Groove-Binding Olioppyrrole Carriers

AUTHOR(S): Baraldi, Pier Giovanni; Balboni, Gianfranco: Cacciari, Barbara; Guiotto, Andrea: Manfrednin; Stefano: Romagnoli, Romeo; Spalluto, Giampiero; Thurston, David E.; Howard, Philip W.; Bianchi, Nicoletta; Rutigliano, Cristina; Mischiati, Carlo; Gambari, Roberto

CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche e Dipartimento di Biochimica e Biologia Molecolare, Universita di Ferrara, Ferrara, 44100, Italy

SOURCE: Journal of Medicinal Chemistry (1999), 42(25), 5131-5141

CODEN: JMCMAR; ISSN: 0022-2623

American Chemical Society

DOUMENT TYPE: Journal

LANGUAGE: JSS949-69-69 256949-70-99

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); SNC (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(Precoass)

(preparation, antiproliferative activity, and DNA-binding pyrrolobenzodiazepines containing oligopyrrole carriers)

N 156949-69-6 HCAPLUS

Absolute stereochemistry.

ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

• HCl

PAGE 1-B

256949-62-9

23594-62-9

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(preparation, antiproliferative activity, and DNA-binding
pyrrolobenzodiazepines containing oligopyrrole carriers)

256949-62-9 HCAPLUS

1H-Pyrrole-2-carboxamide, N-[5-[[[5-[[(3-amino-3iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1methyl-1H-pyrrol-2-yl]-5-[[(5-amino-1-methyl-1H-pyrrol-2yl]carbonyl]amino]-1-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

• HC1

PAGE 1-B

256949-70-9 HCAPLUS

1H-Pyrrole-2-carboxamide, N-[5-[[[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-5-[[[1-ax-3-[[(1laS)-2,3,5,1la-tetrahydro-7-methoxy-5-oxo-1H-pyrrolo[2,1-c][1,4]benzodiazepin-8-yl]oxylpropyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-, monohydrochloride

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

PAGE 1-A

●2 HC1

PAGE 1-B

— сн₂— с- мн₂

256949-61-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation, antiproliferative activity, and DNA-binding
pyrrolobenzodiazepines containing oligopyrrole carriers)
256949-61-8 HCAPUS
1H-Pyrrola-2-carboxamide, N-[5-[[(3-amino-3-iminopropy)]amino]carbonyl}-1methyl-1H-pyrrol-3-yl]-5-[[(5-amino-1-methyl-1H-pyrrol-2yl)carbonyl]amino]-1-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

256949-65-2P 256949-66-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation, antiproliferative activity, and DNA-binding pyrrolobenzodiazepines containing oligopyrrole carriers)

ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 256949-65-2 MCAPLUS | H-Pyrrolo[2,1-c][1,4]benzodiazepine-10(5H)-carboxylic acid, B-[3-[[5-[[5-[[5-[[5-[1,4]mino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino[carbonyl]-1-methyl-1H-pyrrol-2-yl]amino[carbonyl]-1-methyl-1H-pyrrol-2-yl]amino[carbonyl]-1-methyl-1H-pyrrol-2-yl]amino[carbonyl]-1-methyl-1H-pyrrol-2-yl]amino[-3-oxopropoxyl]-2,3,11,1la-tetrahydro-1l-hydroxy-7-methoxy-5-oxo-, 2,2,2-trichloroethyl ester, monohydrochloride, (115,11aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

256949-66-3 HCAPLUS

1H-Pyrrolo[2,1-c][1,4]benzodiazepine-10[5H)-carboxylic acid,

8-[3-[[5-[[5-[[5-[[5-[([5-[(3-amino-3-iminopropy])amino]carbonyl]-1-methyl1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1
methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]-3
coxpropoxyl-2,3,11,1la-tetrahydro-1l-hydroxy-7-methoxy-5-oxo-,
2,2,2-trichloroethyl ester, monohydrochloride, (11S,11aS)- (9CI) (CA

INDEX NAME) INDEX NAME)

Absolute stereochemistry.

ANSWER 15 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: $26\ \mathrm{Aug}\ 1998$

$$\begin{array}{c|c} CH_2O & & \\ & & \\ & & \\ Ph & \\ &$$

AB The title compds., e.g. I [R1 represents optionally substituted aralkyl, etc.: Z represents optionally alkylated nitrogen, etc.; X1 represents CHZNNCO, etc.: X2 represents phenylene, etc.; X3 represents a single bond, etc.: Y2 represents optionally substituted aryl, etc.: and B represents oxygen, etc.], are prepared In an in vitro test for cPLA2 inhibition, the title compound II showed IC50 of 0.17 mM.

ACCESSION NUMBER: 1998:543071 HCAPLUS
DOCUMENT NUMBER: 129:161558
TITLE: Preparation and formulation of thiazolidinedione derivatives as phospholiage A2 inhibitors.

129:161558
Preparation and formulation of thiazolidinedione derivatives as phospholipase A2 inhibitors
Seno, Kaoru; Ohtani, Mitsuaki; Watanabe, Fumihiko Shionogi 4 Co., Ltd., Japan
PCT Int. Appl., 178 pp.
CODEN: PIXXD2
Patent INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: Patent Japanese

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA'	FENT	NO.			KIN	D	DATE		- 1	APPL	ICAT	ION	NO.		D.	ATE	
						-									-		
WO	9833	797			A1		1998	0806	1	WO 1	998-	JP30	7		1	9980	127
	W:	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,
		DK,	EE,	ES,	FI,	GB,	GE,	GH,	GM,	G₩,	Hυ,	ID,	IL,	IS,	JP,	KE,	KG,
		KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,
		NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	UA,
		UG,	US,	υz,	٧N,	YU,	ZW,	AM,	ΑZ,	BY,	KG,	ΚŻ,	MD,	RU,	TJ,	TM	
	RW:	GH,	GM,	KE,	LS,	MW,	SD,	SZ,	UG,	ZW,	AT,	BE,	CH,	DE,	DK,	ES,	FI,
		FR,	GΒ,	GR,	ΙE,	ΙT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,
		GΑ,	GN,	ML,	MR,	NE,	SN,	TD,	TG								
T₩	5778	75			В		2004	0301		TW 1	998-	8710	1064		1	9980	126
CA	2277	947			AA		1998	0806		CA 1	998-	2277	947		1	9980	127
CA	2277	947			C		2004	0921									

Page 2330/08/2005

ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

REFERENCE COUNT:

39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L	3 ANS	WER	15 O	F 41	HCF	APLUS	COPYRIGH	T 2005	ACS o	n STN		(Cor	ntin	ued)	
	AU	9855	775			A1	1998082	5 AU	1998	-5577	5		1	9980	127
	ΑU	7192	10			B2	2000050	14							
	BR	9807	132			A	2000012	.5 BR	1998	7132			1	9980	127
	EP	9767	48			A1	2000020)2 EP	1998	-9007	41		1	9980	127
	EP	9767	48			В1	2003120	13							
		R:	AT,	BE,	CH,	DE,	DK, ES, FE	R, GB, G	R, I1	, LI,	LU,	NL,	SE,	MC,	PT,
			ΙE,	FI											
	TR	9901	847			T2	2000062	1 TR	1999	9901	847			9980	
	RU	2198	174			C2	2003021	O RU	1999	+1194	81			9980	
	AT	2555	79			E	200312	15 AT	1998	-9007	41			9980	
	PT	9767	48			T	2004033	31 PT	1998	-9007	41			9980	
	ES	2210	710			Т3	2004070)1 ES	1998	9007	41			9980	
	US	6147	100			A	2000111	4 US	1999	-3550	08		1	9990	722
	NO	9903	706			A	1999093	O NO	1999	-3706			1	9990	729
	NO	3138	81			B1	2002121	16							
	MX	9907	061			A	2000022	28 MCX	1999	-7061			1	9990	729
P	RIORITY	APP	LN.	INFO	. :			JP	1997	-1796	2	,	۹ 1	9970	131
								WC	1998	3-JP30	7	,	7 1	9980	127

OTHER SOURCE(S):

R SOURCE(S): MARPAT 129:161558
211297-31-3P 211297-34-6P 211298-04-3P
211298-06-5P
REL: BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SPN (Synthetic preparation): TMU (Therapeutic use): BIOL (Biological study): PREP (Preparation): USES (Uses)
(preparation of thiazolidinedione derivs. as phospholipase A2 inhibitors)
21297-31-3 HCAPLUS
2-Pyrrolidinecarboxamide, 4-([1,1'-biphenyl]-2-ylmethoxy)-1-[2-(4-fluorobenzoyl)benzoyl]-N-[5-(4-oxo-2-thioxo-5-thiazolidinylidene)methyl]2-thienyl]-, (2S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

211297-34-6 HCAPLUS 2-Pyrrolidinecarboxamide, 4-([1,1'-bipheny1]-2-ylmethoxy)-N-[5-[(2,4-dioxo-5-thiazolidinylidene)methyl]-2-thienyl]-1-[2-(4-methylbenzoyl)benzoyl]-, (25,4R)- (9CI) (CA INDEX NAME)

ANSWER 15 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) Absolute stereochemistry. Double bond geometry unknown.

211298-04-3 HCAPLUS 2-Pyrrolidinecarboxamide, 4-{([1,1'-biphenyl]-2-ylmethyl)thio}-N-[5-{(2,4-dioxo-5-thiazolidinylidene)methyl]-2-thienyl]-1-{2-(4-fluorobenzoyl)benzoyl}-, (2S,4R}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

ANSWER 15 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)
1-Pyrrolidinecarboxylic acid, 4-([1,1'-biphenyl]-2-ylmethoxy)-2-([[5-[(2,4-dioxo-5-thiazolidinylidene)methyl]-2-thienyl]amino]carbonyl]-,
1,1-dimethylethyl ester, (2S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 15 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

211298-06-5 HCAPLUS 2-Pyrrolidinecarboxamide, $4-[(\{1,1'-biphenyi\}^-2-ylmethyl)thio\}-1-\{2-\{4-fluorobenzoyl\}-bnzoyl\}-N-\{5-\{\{4-oxo-2-thioxo-5-thiazolidinylidene)methyl\}-2-thienyl\}-, (2S,4R)- (9CI) (CA INDEX NAME)$

Absolute stereochemistry.
Double bond geometry unknown.

IT 211298-68-9P 211298-69-0P

RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of thiazolidinedione derivs. as phospholipase A2 inhibitors) 211298-68-9 HCAPLUS

(preparation of the action of the control of the co (CA INDEX NAME)

Absolute stereochemistry.

211298-69-0 HCAPLUS

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 20 Aug 1997

A new upper limit of binding site size is defined for the hairpin polyamide-DNA motif. Ten-ring hairpin polyamides containing pyrrole (Py) and imidazole (Im) amino acids were designed for recognition of seven base pair (bp) sequences in the minor groove of DNA. The DNA binding properties of two polyamides, ImplypyPyPy-P-Dp, and ImImPyPyPy-Y-ImPyPyPyPy-B-Dp were analyzed by footprinting and affinity cleavage on a DNA fragment containing the resp. match sites 5'-TGTARCA-3' and 5'-TGGARCA-3'. Quant. footprint titrns. demonstrate that ImpPyPyPy-Y-ImpPyPyPy-B-Dp binds the 7-bp match sequence 5'-TGTARCA-3' with an equilibrium association constant (Ka) of Ka = 1.2 + 1010 M-1 and 18-fold specificity vs. the single base pair mismatch sequence 5'-TGGARCA-3'. ImImPyPyPyPy-P-Dp by a single amino acid substitution and binds its match 5'-TGGARCA-3' site with Ka = 3.6 + 109 M-1 and 300-fold specificity vs. its corresponding single base pair mismatch sequence 5'-TGTARCA-3'. Ten-ring hairpin polyamides have binding affinities similar to those of eight-ring hairpin polyamides. These results indicate that the affinity of hairpin binding ceases to increase as the length of the polyamide subunits increases beyond four rings, analogous to the behavior of unlinked subunits. Therefore, recognition of seven base pairs by a ten-ring hairpin polyamide most likely represents an upper limit to the effective targetable site size of the hairpin polyamide-DNA motif.

ACCESSION NUMBER: 1997:528757 HCAPLUS

ENCLOPENT NUMBER: 17:216506

Recognition of Seven Base Pair Sequences in the Minor Groove of DNA by Ten-Ring Pyrrole-Imidazole Polyamide Hairpins

127:216506 Recognition of Seven Base Pair Sequences in the Minor Groove of DNA by Ten-Ring Pyrrole-Imidazole Polyamide

Groove of DNA by Ten-Ring Pyrrole-Imidazole Polyamic Hairpins
Turner, James M.; Baird, Eldon E.; Dervan, Peter B. Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, 91125, USA
Journal of the American Chemical Society (1997), 119(33), 7636-7644
CODEN: JACSAT; ISSN: 0002-7863
American Chemical Society
Journal AUTHOR (S): CORPORATE SOURCE:

SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE: IT 194857-41-Journal

ISHAN: American Chemical Society
MENT TYPE: Journal
UAGE: English
194857-41-5P 194857-42-6P
RL: BPR (Biological process): BSU (Biological study, unclassified); CAT
(Catalyst use): SPN (Synthetic preparation): BIOL (Biological study): PREP
(Preparation): PROC (Process): USES (Uses)
(preparation of and recognition of seven base pair sequences in the minor
groove of DNA by ten-ring pyrrole-imidazole polyamide hairpins)
Iron, (2, 3, 4, 5-tetradehydro-1-methyl-4-[[[1-methyl-4-[1-methyl-4-[1-m

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

PAGE 1-C

(Continued)

PAGE 2-A

ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

PAGE 2-B

(Continued)

PAGE 2-C

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

(Continued)

PAGE 2-B

PAGE 2-C

194857-40-4P 194857-49-3P 194857-50-6P RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(Process)

(proparation of and recognition of seven base pair sequences in the minor groove of DNA by ten-ring pyrrole-imidazole polyamide hairpins)

194857-40-4 HCAPLUS

H-Imidazole-2-carboxamide, 1-methyl-4-[[(1-methyl-1-H-imidazol-2-yl)carbonyl]amino]-N-[1-methyl-5-[[[1-methyl-5-[[[1-methyl-5-[[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[1-methyl-5-[[1-methyl-5-[1-methyl-5-[[1-methyl-5-[1-methyl-5-[1-methyl-5-[[1-methyl-5-[1-methyl-5-[1-methyl-5-[[1-methyl-5-[1-methyl-5-[1-methyl-5-[[1-methyl-5-[1-methyl-

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-C

- (CH2) 3 - NHMe

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-C

PAGE 2-A

194857-50-6 HCAPLUS
B-Alaninamide, 2,3,4,5-tetradehydro-1-methyl-4-[{[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[1]]]]]]]]]]
methyl-4-[[[1-methyl-4-[[1-methyl-1H-imidazol-2-yl]]amino]-1H-purol-2-yl][arbonyl]amino]-1H-pyrrol-2-yl][arbonyl]amino]-

LB ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

 $\label{eq:continuous} $$194857-49-3$$$ HCAPLUS $$\beta-Alaninamide, 2,3,4,5-tetradehydro-1-methyl-4-[[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-methyl-4-methyl-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]-M-[1-methyl]-4-methyl]-4-methyl]-9-oxo-4,8,11,14-tetraazapentadec-1-yl]-(9CI) (CA INDEX NAME)$

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-C

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

194857-46-0DP, conjugates with Pam resin 194857-47-1P
194857-48-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of and recognition of seven base pair sequences in the minor
groove of DNA by ten-ring pyrrole-imidazole polyamide hairpins)
194857-46-0 HCAPLUS
B-Rlanine, 2, 3, 4, 5-tetradehydro-1-methyl-4-[[[1-methyl-4-[[[1-methyl-4-[[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[1]]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-C

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

(Continued)

194857-47-1 HCAPLUS

1H-Imidazole-2-carboxamide, N-[5-[[[5-[[5-[[5-[[3-[[3-[(3-aminopropy]] amino] carbonyl]-1-methyl-1H-pyrrol-2-yl] amino] carbonyl]-1-methyl-1H-pyrrol-2-yl] amino] carbonyl]-1-methyl-1H-pyrrol-2-yl] amino] carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-4-[[4-[[4-[t]-methyl-4-[[1-methyl-4-[[1-methyl-4-[1-d-[t]-methyl-4-[t]-d-[t]-methyl-4-[t]-methyl-4-[t]-methyl-4-[t]-methyl-4-[t]-methyl-4-[t]-methyl-4-[t]-methyl-4-[t]-methyl-4-[t]-methyl-1-met

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

(Continued)

PAGE 1-C

-- (CH2) 3-NH- (CH2) 3-NH2

PAGE 2-A

PAGE 1-C

- (CH2) 3-NH- (CH2) 3-NH2

ANSWER 17 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 27 Apr 1996

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention is directed to novel cyclopropylpyrroloindole-oligopeptide compds. Which are useful as anticancer agents. The novel cyclopropylpyrroloindole-oligopeptide compds. However, the properties of t

123:1148U
Cyclopropapyrroloindole-oligopeptide anticancer agents
Lown, J. William: Wang, Yuqiang; Luo, Weide
Symphar Laboratories, Inc., Can.
U.S., 17 pp.
CODEN: USXXAM

DOCUMENT TYPE: English FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PAT	TENT	NO.			KIN	D	DATE			APP	LICA	τI	ON I	ю.		D.	ATE		
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US	5502	068			А		1996	0326		US	1995	- 3	813	55		1	9950	131	
CA	2210	093			AA		1996	8080		CA	199€	- 2	2100	93		1	9960	131	
WO	9623	497			A1		1996	8080		WO	199€	i-L	1572	7		1	9960	131	
	W:	AL,	AM,	AT,	AU,	AZ,	BB,	BG,	BR,	BY	, CA	١,	CH,	CN.	cz.	DE.	DK.	EE,	
		ES,	FI,	GB,	GE,	ΗŲ,	IS,	JP,	KE,	KG	, KE	٠,	KR.	KZ.	LK.	LR.	LS.	LT.	
							MN,												
		SG,													-				
	RW:	KE,	LS,	MW,	SD,	SZ,	UG,	AT,	BE,	CH	, DE	:.	DK.	ES.	FR.	GB.	GR.	IE,	
							SE,												NE
ΑU	9649				A1		1996												
ΑU	6980	01			B2		1998	1022											
EP	8003	90			A1		1997	1015		ĘΡ	199€	, - g	061	76		1	9960	131	
EP	8003	90			В1		2002	1204											
	R:	AT,	BE,	CH,	DΕ,	DK,	ES,	FR,	GB,	GR	. 11	٠.	LI.	LU.	NL.	SE.	MC.	PT.	ΙE

Page 2830/08/2005

LB ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

REFERENCE COUNT:

THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HELLIN THE PARTY.

ANSWER 18 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 23 Dec 1995

AB Novel aminoalkyl substituted indolocarbazoles I {R = Q1 (n = 1, 2, 3), HN(CH2)3NMe2, etc.} were prepared from staurosporine aglycon and characterized with respect to inhibition of protein kinases C and A. In both series, potent and selective PKC inhibitors could be identified. Structure activity relationships are discussed.

ACCESSION NUMBER: 1995:1002143 HCAPLUS

DOCUMENT NUMBER: 124:175641

Novel substituted indolocarbazoles as potent and selective inhibitors of protein kinase C

AUTHOR(S): Xie, Guojan: Nagata, Hiroyuki: Tamaoki, Tatsuya; Lown, J. William

CORPORATE SOURCE: Dep. Chem., Univ. Alberta, Alberta, T6G 2G2, Can. Bicorganic 4 Medicinal Chemistry Letters (1995), 5(23), 2841-4 CODEN: BNCLE8: ISSN: 0960-894X

PUBLISHER: DOCUMENT TYPE: Jaurnal

PUBLISHER: CUDEN: E Elsevier DOCUMENT TYPE: Journal LANGUAGE: English IT 173917-98-1F 173917-99-2P

173917-98-1P 173917-99-2P
RL: BRC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation and protein kinase inhibitory activity of indolocarbazoles) 173917-98-1 HCAPLUS
H-Pyrrole-2-carboxylic acid, 1-methyl-5-[{[1-methyl-5-{[1-oxo-3-(5,6,7,13-tetrahydro-7-oxo-12H-1ndolo[2,3-a]pyrrolo[3,4-c]carbazol-12-yl]propyl]amino]-H-pyrrol-2-yl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

L8 ANSWER 18 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

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173917-95-9 173917-96-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and protein kinase inhibitory activity of indolocarbazoles)
173917-95-8 HCAPLUS
H-Pyrrole-2-carboxylic acid, 5-[[(5-amino-1-methyl-1H-pyrrol-2yllcarbonyllamino|-1-methyl-, methyl ester (9CI) (CA INDEX NAME)

L8 ANSWER 18 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

173917-99-2 HCAPLUS

1H-Pytrole-2-carboxylic acid, 1-methyl-5-[[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[1-methyl-5-[1-methyl-5-[1-methyl-5-[1-methyl-5-[1-methyl-5-[1-methyl-5-]]]]

12-yl)propyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-pytrol-2-yl)carbonyl|amino|-1H-p

L8 ANSWER 18 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

173917-96-9 HCAPLUS
1H-Pyrrole-Z-carboxylic acid, 5-{[[5-{[[5-amino-1-methyl-lH-pyrrol-2-yl)carbonyl]amino]-1-methyl-lH-pyrrol-2-yl]carbonyl]amino]-1-methyl-methyl ester [9C1] (CA IMDEX NAME)

ANSWER 19 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 14 Dec 1995

AB Title compds. [I; Rl = H, halo, alkyl, alkoxy, etc.; R2 = (acyl)alkyl, acyl. CH:CHCO2H, etc.; R3 = H, alkyl, CH2Ph; R4 = SH, SnR, SeH, SenR, etc.; R = H, alkyl, (heterolaryl, I in which R4 = bond, etc.; R4R5 = S, Se; R5R6 = bond; R6 = H; n = 1-3] were prepared 2Hus, I-methyl-2-indolinone was treated with P2SS and the product condensed with PhNCO to give, after oxidation, title compound II which had IC50 of 3-4µM against growth factor mediated mitogenesis in vitro.

ACCESSION NUMBER: 1995:9812554 HCAPLUS
DOCUMENT NUMBER: 1995:9812554 HCAPLUS
TITLE: Preparation of 2-indolyldisulfides and analogs as protein tyrosine kinase inhibitors and antitumor agents
INVENTOR(S): Dobrusin, Ellen M.; Showalter, Howard D. H.; Denny, William A.; Palmer, Brian D.; Rewcastle, Gordon W.; Tercel, Moana; Thompson, Andrew M.

PATENT ASSIGNEE(S): Warner-Lambert Co., USA
U.S., 53 pp. Cont.-in-part of U.S. Ser. No. 926, 015, abandoned.
CODEN: USXXAW
DOCUMENT TYPE: Patent
LANGUAGE: English

INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: FACE. FACE. English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5464861	Α	19951107	US 1993-94792	19930809
HU 71553	A2	19951228	HU 1995-341	19930802
CZ 283965	В6	19980715	CZ 1995-288	19930802
NZ 255194	А	20000128	NZ 1993-255194	19930802
US 5556874	Α	19960917	US 1995-438616	19950510
PRIORITY APPLN. INFO.:			US 1992-926015 B	2 19920806
			US 1993-94792 A	3 19930809

OTHER SOURCE(S): MARPAT 124:175826

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

EM ANSWER 20 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 10 Jan 1995

BA a series of 3 -substituted 2,2'-dithiobis(lH-indoles) were synthesized and evaluated for their ability to inhibit the tyrosine kinase activity of both the epidermal growth factor receptor (EGFR) and the nonreceptor pp60v-src tyrosine kinase, to extend the available structure-activity relationships for this series. The majority of the compds. were prepared either by reaction of 2-chloro-1-methylindole-3-carbonyl chloride with amines, followed by thlomethylation, demethylation, and oxidative dimerization, or by reaction of isocyanates with the anion of 1-methyl-2-indointehione followed by dimerization. Overall, inhibitory activity is realizated by analogs having a wide variety of side chains. A series of 3-carboxamide analogs had moderate to good activity against isolated EGFR (ICS0s 1-20 µM), with monoalkyl substitution of the carboxamide being optimal. Polar side chains were generally less effective than lipophilic ones, with benzyl being particularly effective. However, N.N-disubstitution was the most effective pattern for inhibition of pp60v-src. A variety of substituted N-phenylcarboxamides had lower activity against EGFR than the parent derivative, and a N-thienylcarboxamide also had low activity. A series of 3-ketones, including Me, Ph, and furyl derivs., showed moderate activity against the pp60v-src kinase, but were less effective against EGFR. The mechanism of inhibition of both kinases by these drugs was shown to be noncompetitive with respect to both ATP and peptide substrate. Selected compds. inhibited the growth of Swiss 3T3 cells with IC50s in the low micromolar range and inhibition of both kinases by these drugs was shown to be noncompetitive with respect to both ATP and peptide substrate. Selected compds. inhibited the growth of Swiss 3T3 cells with IC50s in the low micromolar range and inhibition is 3T3 cells with IC50s in the low micromolar range and inhibition of both kinases inhibition in thiol-disulgide exc

DOCUMENT NUMBER: TITLE:

1995:283368 HCAPLUS
123:248
Tyrosine Kinase Inhibitors. 4. Structure-Activity
Relationships among N- and 3-Substituted
2,2'-Dithiobis(1H-indoles) for in vitro Inhibition of
Receptor and Nonreceptor Protein Tyrosine Kinases
Palmer, Brian D.; Rewcastle, Gordon W.; Thompson,
Andrew M.; Boyd, Maruta; Showalter, H. D. Hollis;
Sercel, Anthony D.; Fry, David W.; Kraker, Alan J.;
Denny, William A.
School of Medicine, University of Auckland, Auckland,
92019, N. Z.
JOURNAI Of Medicinal Chemistry (1995), 38(1), 58-67
CODEN: JMCMAR; ISSN: 0022-2623
American Chemical Society
Journal English AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

156136-37-7P

136136-37-79
RE: BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SPN (Synthetic preparation); BIOL (Biological study): PREP (Preparation)
(structure-activity relationships among dithiobisindoles for inhibition of receptor and nonreceptor protein tyrosine kinases)
156136-37-7 HCAPLUS
1H-Indole-3-carboxamide, 2,2'-dithiobis(1-methyl-N-2-thienyl- (9CI) (CA INDEX NAME)

INDEX NAME

ANSWER 19 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of Z-indolyldisulfides and analogs as protein tyrosine kinase inhibitors and antitumor agents) 156136-37-7 HCAPLUS HT-Indole-3-carboxamide, 2,2'-dithiobis[1-methyl-N-2-thienyl- (9CI) (CAINDRY NAME)

L8 ANSWER 20 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

EN ANSWER 21 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN
Entered STN: 17 Nov 1994

AB In the present study, the authors have investigated the effect of unprecedented chemical modifications introduced in the distamycin mol., with the aim of assessing their ability to interfere with sequence-specific DNA-protein interactions in vitro. By using an electrophoretic mobility shift assay, the authors have been able to identify novel distamycin analogs with improved displacing abilities on the binding of octamer nuclear factors to their target DNA sequence. While variations in the number of pyrrole rings and/or reversion of an internal amide bond result in distamycin—like compds. with identical or very simular properties, the reversion of the formamido into a carboxyamido group or its replacement with the charged formimidoyl moiety significantly improves the ability of the resulting novel distamycin derive, to compete with OCT-1 (octamer 1 nuclear factor) for its target DNA sequence. Tissue-specific octamer-dependent in vitro transcription is similarly affected by these chemical modifications, suggesting that the ability of distamycins to bind octamer sequences has a direct influence on the functional state of octamer-containing promoters. These data represent an initial, successful attempt to rationalize the design of DNA binding drugs, using distamycins as a model.

ACCESS FOR NOMBER: 1995:199500 HCAPLUS
DOCUMENT NUMBER: 122:45671

attempt to rationalize the design of DNA binding drugs, using distamycins as a model.

ACCESSION NUMBER: 1995:199500 HCAPLUS
DOCUMENT NUMBER: 122:45671
TITLE: Distamycin analogs with improved sequence-specific DNA binding activities

AUTHOR(S): Clucci, Alessandra; Feriotto, Giordana; Mischiati, Carlo; Gambari, Roberto; Animati, Fabio; Lombardi, Paolo; Natali, Pier Giorgio; Arcamone, Federico; Giacomini, Patrizio

CORPORATE SOURCE: Menarini Ricerche Sud, Italy
SOURCE: Biochemical Pharmacology (1994), 48(8), 1583-91
CODENT TYPE: Journal
LANGUAGE: Elsevier

LOCUMENT TYPE: Journal
LANGUAGE: English
IT 159565-63-6, MEN 10398 159565-64-7, MEN 10557

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(distamycin analogs with improved sequence-specific DNA binding activities)

RN 159565-63-6 HCAPLUS

CN 1H-PYCRO1e-2, 4-dicarboxamide, N2-(3-amino-3-iminopropyl)-N4-[4-[[4-(formylamino)-1-methyl-1H-pyrro1-2-yl]-arbonyl]amino)-1-methyl-1H-pyrro1-2-yl]-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 22 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 10 Dec 1994

AB Title compds. I (A = (substituted) Ph or thienyl: R1 = MeCH(OH), MeCHF, HOCH2: R2 = H, C1-4 alkyl: R3, R4 = H, halo, NC, C1-4 alkyl, O2N, HO, HO2C, C1-4 alkoxy, F3C, etc.:x = c1-6 alkanediyl interrupted by O, S(O)x wherein x = 0-2, RSNCO wherein x = 0-2, RSCO wherein x = 0-2, R

INVENTOR (S):

121:280467
Preparation of antibiotic carbapenem compounds
Betts, Michael John; Davies, Gareth Morse; Jung,
Frederic Henri
Zeneca Ltd., UK; Zeneca Pharma S.A.
Eur. Pat. Appl., 27 pp.
CODEN: EPEXXDW
Patent

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
EP 590885	A1 19940406	EP 1993-307551	19930923
EP 590885	B1 20000315		
R: AT, BE, CH,	DE, DK, ES, FR, C	B, GR, IE, IT, LI, D	U, MC, NL, PT, SE
CA 2106141	AA 19940329	CA 1993-2106141	19930914
US 5527791	A 19960618	US 1993-123998	19930921
AT 190615	E 20000415	AT 1993-307551	19930923
ES 2144446	T3 20000616	ES 1993-307551	19930923
JP 06211860	A2 19940802	JP 1993-241519	19930928
PRIORITY APPLN. INFO.:		EP 1992-402648	A 19920928
OTHER SOURCE(S):	MARPAT 121:280467	,	
IT 154308-86-8P 154308-	87-9P 158743-30-7P		

154308-86-8P 154308-87-9P 158743-30-7P
158743-31-3P 158743-32-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of carbapenem antibiotics)
154308-86-8 HCAPIUS
154308-86-8 HCAPIUS
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[[5-[2-propenyloxy)carbonyl]-2-thienyl]amino]carbonyl]-, (4-nitrophenyl)methyl ester, (25-cis)- (9CI) (CA INDEX NAME)

Page 3130/08/2005

ANSWER 21 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

159565-64-7 HCAPLUS
1H-Pyrrole-2,4-dicarboxamide, N4-[4-[{[4-{aminocarbonyl}-1-methyl-1H-pyrrol-2-yl]-n2-(3-amino-3-iminopropyl}-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L8 ANSWER 22 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) Absolute stereochemistry.

154308-87-9 HCAPLUS

19430-07-9 notebook | 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[(5-carboxy-2-thienyl)amino[carbonyl]-, 1-[(4-nitrophenyl)methyl] ester, (25-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

158743-30-7 HCAPLUS

lagrassur merkus 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[[5-[[(carboxymethyl)amino]carbonyl]-2-thienyl]amino]carbonyl]-, 1-[(4-nitrophenyl)aethyl] ester, (28-cia)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

158743-31-8 HCAPLUS 130743-31-0 increases
1-Pyrrolidinecarboxylic acid, 2-[[[5-[[(carboxymethyl)amino]carbonyl]-2thienyl]amino]carbonyl]-4-mercapto-, 1-[(4-nitrophenyl)methyl] ester,
(23-cia)-[9C1] (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 22 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

158743-32-9 HCAPLUS
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[5-[[5-[[(a-toxpmethyl) amino]carbonyl]-2-thienyl]amino]carbonyl]-1-[((4-nitrophenyl)methoxy]carbonyl]-3-pyrrolidinyl]thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 2-[(4-nitrophenyl)methyl] ester, [4R-[3(35*,55*),4q,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

LB $\,$ ANSWER 23 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Absolute stereochemistry. (Continued)

155481-44-0 HCAPLUS
1-Pyrrolidinecarboxylic acid, 4-mercapto-2-{([5-{(2-propenyloxy)carbonyl}2-thienyl]amino}carbonyl}-, (4-nitrophenyl)methyl ester, (2S-cis)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

156631-45-7 HCAPLUS

13661-43-7 RAPLUS
4-Thia-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid,
6-[1-[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]-3-[[1-[(4nitrophenyl)methoxylcarbonyl]-5-[[[5-[(2-propenyloxy)carbonyl]-2thienyl]mmino[carbonyl]-3-pyrrolidinyl[thio]-7-oxo-, 2-propenyl ester,
[58-[3](35-), 55-), 56, 64[8^+]]- [90]) (CA INDEX NAME)

Absolute stereochemistry.

Page 3230/08/2005

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PA	TEN	T	NO.			KIND)	DATE			APE	LICA	TION	I NO			D.	ATE		
																		-			
	EP	59	21	67			Al		1994	0413		EΡ	1993	-307	843			1	9931	001	
	EP	59	21	67			B1		1999	1222											
		R	:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GF	, IE	, IT	, L	Ι,	LU,	MC,	NL,	PT,	SE
	CA	21	06	330			AA		1994	0408		CA	1993	-210	633	0		1	9930	916	
	AT	18	79	68			E		2000	0115		ΑT	1993	-307	843			1	9931	001	
	ĖS	21	40	445			T3		2000	0301		ES	1993	-307	843			1	9931	001	
	JP	06	21	1871			A2		1994	0802		JР	1993	-250	437			1	9931	006	
	US	55	38	962			A		1996	0723		US	1993	-132	256			1	9931	006	
RIO	RIT	ΥA	PP	LN.	INFO	. :						EΡ	1992	-402	733			A 1	9921	007	
THE	R S	OUR	CE	(S):			MARE	TA	121:	1083	68										

R SOURCE(S): MARPAT 121:108368
154308-86-0P 155681-44-0P 156631-45-7P
156631-46-0P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antibiotics)
154308-86-8 HCAPLUS
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[5-[(2-propenyloxy)carbonyl]-2-thienyl]amino]carbonyl]-, (4-nitrophenyl)methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

ANSWER 23 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

156631-46-8 HCAPLUS

136531-40-8 HCAPLUS
4-Thia-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid,
6-(1-hydroxyethyl)-3-[[1-[[(4-nitrophenyl)methoxy|carbonyl]-5-[[[5-[(2-propenyloxy)carbonyl)-2-thienyl]aminolcarbonyl]-3-pyrcolidinyl]thio]-7-oxo-,
2-propenyl ester, [5R-[3(33*,55*),5α,6α(R*)]]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 24 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 03 Sep 1994
A simple 10-membered monocyclic 3-ene-1,5-diyne has been prepared tethered to a derivative of netropsin. It is proposed that the attachment to this reactive diyne-ene to a mol. which assocs. with B-DNA in the minor groove can enhance the potency of the diyne-ene as a DNA cleavage agent. The nature of the tether appears to be very important in the magnitude of this enhancement, based on two examples reported here. With a two-carbon tether, there is a small increase in DNA cleavage compared with the parent diyne-ene. However, a four-carbon tether, based on a crotonate linkage, shows almost a 2000-fold enhancement of the parent diyne-ene. DNA blinding studies using CD measurements and ethidium bromide displacement show that the relative binding constant of the diyne-ene and the two versions tethered to netropsin parallel the DNA cleavage effectiveness.

ACCESSION NUMBER: 1994:49071 RACPLUS

DOCUMENT NUMBER: 121:99071

TITLE: The Effect on DNA Cleavage Potency of Tethering a Simple Cyclic Enediyne to a Netropsin Analog

AUTHOR(S): Semmelhack, M. F., Gallagher, J. J.; Ding, W.-d.; Krishnamurthy, G., Babine, R.; Ellestad, G. A.

CORPORATE SOURCE: Department of Chemistry, Princeton University, Princeton, NJ, 08544, USA

SOURCE: Journal of Organic Chemistry (1994), 59(16), 4357-9

DOCUMENT TYPE: Journal of Organic Chemistry (1994), 59(16), 4357-9

DOCUMENT TYPE: Journal of Organic Chemistry (1994), 59(16), 4357-9

DOCUMENT TYPE: Journal of Organic Chemistry (1994), 59(16), 4357-9

DOCUMENT TYPE: Journal of Organic Chemistry (1994), 59(16), 4357-9

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DOCUMENT TYPE: Journal of Organic Chemistry (1994), 59(16), 4357-9

DOCUMENT TYPE: Journal Of Organic Chemistry (1994), 59(16), 4357-9

DOCUMENT TYPE: Journal Of Organic Chemistry (1994), 59(16), 4357-9

DOCUMENT TYPE: Journal Of Organic Chemistry (1994), 59(16), 4357-9

DOCUMENT TYPE: Journal Of Organic Chemistry (1994), 59(16), LANGUAGE: IT 156055-65-1 186055-65-1
RK: BIOL (Biological study)
(DNA-cleaving activity of and reaction with monocyclic enediynes of, structure in relation to)
156055-65-1 HCAPUS
1H-Pyrrole-2-carboxamide, 4-amino-N-[5-[{(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl}-1-methyl- (9CI) (CA INDEX NAME) 156055-66-2P 156055-69-5P 156055-66-29 156055-69-59

RE: SPN (Synthetic preparation); PREP (Preparation)
(preparation and DNA-cleaving activity of, structure in relation to)
156055-66-2 HCAPLUS
Acetic acid, (4-cyclododecene-2,6-diyn-1-yloxy)-, compd. with
4-amino-N-[5-[[(3-amino-3-iminopcopyl) amino]carbonyl]-1-methyl-1H-pyrrol-2yl]-1-methyl-1H-pyrrole-2-carboxamide (1:1) (9CI) (CA INDEX NAME) CM 1 CRN 156055-65-1 CMF C15 H21 N7 O2

ANSWER 24 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ANSWER 24 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 2 CRN 156055+64-0 CMF C14 H16 03 сн₂-- со₂н 156055-69-5 HCAPLUS
2-Butenoic acid, 4-(4-cyclododecene-2,6-diyn-1-yloxy)-, compd. with
4-(13-amino-3-imino-1-oxopropyl)aminol-N-[5-[(3-amino-3-iminopropyl)amino|carbonyl)-1-methyl-1H-pyrrol-2-yl)-1-methyl-1H-pyrrol-2-crboxamide (1:1) (901) (CA INDEX NAME) СМ 2 CRN 156055-67-3 CMF C16 H18 O3 о- сн2- сн= сн- со2н ANSWER 25 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 20 Aug 1994 AB Title compds. [I; Rl = H, halo, OH, alkyl, alkoxy, CO2H, etc.; l or 2 CRl
= N; R2 = (acyl)alkyl, CH:CKCO2H, alkylcarbabamoyl, acyl, etc.; R3 = H,
alkyl, CH2Ph; R4 = ZH, ZNX, ZnQ; R5 = H and R4R6 = S or Se; R5R6 = bond; Q = I in which R4 = Zn and R5R6 = bond; X = H, alkyl, CH2Ph, (heterolaryl; 2 = S, Se; n = 0-3] were prepared Thus, l-methyl-2-indolinone was treated with P2SS and the product treated with NaH and PhNCO to give indolinethionecarboxamide II which had IC50 of 2µM against epidermal growth factor mediated mitogenisis.

ACCESSION NUMBER: 1994:483305 HCAPLUS
DOCUMENT NUMBER: 121:83050
TITLE: 1994:483305 HCAPLUS
INVENTOR(S): 201:83050
Preparation of 2-indolinethiones and related disulfides and seleno-analogs as protein tyrosine kinase inhibitors and antitumor agents
INVENTOR(S): Dobrusin, Ellen Myra: Showalter, Howard Daniel Hollis; Denny, William Alexander; Palmer, Brian Desmond; Rewcastle, Gordon William; Tercel, Moana; Thompson, Andrew Mark
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
PCT Int. Appl., 212 pp.
COODEN: PIXXD2
PALENT DOCUMENT TYPE: English 2 FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE A1 WO 1993-US7272 19940217 WO 9403427 19930802 WO 9403427 AI 19940217 WO 1993-US7272 19930802 W: AU, CA, CZ, FI, HU, JP, KR, NO, NZ, RU, SK RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, NC, NL, PT, SE EP 654024 AI 19950524 EP 1993-918594 19930802 EP 654024 Al 19950524 EP 1993-918594 19930802 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, HU 71553 A2 19951228 HU 1995-341 19930802 JP 08503450 T2 19960926 JP 1993-519671 19930802 AU 672224 B2 19960926 AU 1993-47994 19930802 HU 71553 JP 08503450 AU 672224 AU 9347994 CZ 283965 NZ 255194 19940303 CZ 1995-288 NZ 1993-255194 RU 1995-108332 SK 1995-135 19980715 20000128 19930802 19930802 19930802 19930802

RU 2155187

SK 283413 PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 121:03050 IT 156136-36-6P 156136-37-7P

20000827

156136-36-6P 156136-37-7P
RL: SPN [Synthetic preparation); PREP (Preparation)
(preparation of, as protein tyrosine kinase inhibitor)
156136-36-6 HCRPUS
HR-Indole-3-carboxamide, 2,2'-dithiobis[N-2-furanyl-1-methyl- (9CI) (CA INDEX NAME)

US 1992-926015 WO 1993-US7272

ANSWER 25 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

156136-37-7 HCAPLUS
1H-Indole-3-carboxamide, 2,2'-dithiobis[1-methyl-N-2-thienyl- (9CI) (CA
HDEX NAME)

L8	ANSWER 26 OF 41	HCAPLUS	COPYRIGHT	2005 ACS on STN	(Continued)
	JP 06508372	T2	19940922	JP 1993-516396	19930324
	JP 3313366	B2	20020812		
	AT 185140	E	19991015	AT 1993-906740	19930324
	ES 2136124	Т3	19991116	ES 1993-906740	19930324
	CA 2108356	С	20040120	CA 1993-210835	6 19930324
	CN 1077957	A	19931103	CN 1993-102800	19930326
	CN 1036713	В	19971217		
	NO 9304264	A	19931125	NO 1993-4264	19931125
	FI 104075	B1	19991115	FI 1993-5245	19931125
	US 5519015	A	19960521	US 1993-142459	19931126
PRI	ORITY APPLN. INFO.	:		EP 1992-400836	A 19920326
				EP 1992-402763	A 19921009
				WO 1993-GB603	A 19930324
OTH	ER SOURCE(S):	MARPA	T 121:9029		
IT	154308-86-8P 1554	81-34-8P	155481-36-0	P	
	155401-37-10 1654	01_30_20	155491-40-6	D	

Absolute stereochemistry.

15548]-34-8 HCAPLUS

1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-(1-hydroxyethyl)-4-methyl-3-[[1-[[(4-nitrophenyl)methoxy]carbonyl]-5-[[[4-[(2-propenyloxy|carbonyl]-2-thienyl]mino[carbonyl]-3-pyrrolidinyl]thio]-7-oxo-, 2-propenyl ester, (4R-[3(38*,58*), 4a,59,68(R*)]]-, compd. with N-ethyl-N-(1-methylethyl)-2-propanamine (1:1) [9CI) (CA INDEX NAME)

CM 1

CRN 155481-33-7 CMF C34 H36 N4 O11 S2

ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 09 Jul 1994

AB Title compds. I [R = (un)substituted carboxythienyl: R1 = CHMeOH, CHMeF, CHZOH: R2, R3 = H, alkyl] were prepared Thus, the carbapenem II was obtained from the diphenylphosphoryloxycarbapenem and the thiol, prepared from 2-thiophenecarboxylic acid and the protected mercaptopyrrolidinecarboxylic acid in 4 steps. II had min. inhibitory concns. against Staphylococcus aureus Oxford 0.125 and Escherichia coli DCO 0.008 µg/mL.

ACCESSION NUMBER: 1994:409029 HCAPLUS

DOCUMENT NUMBER: TITLE:

1994:409029 HCAPLUS
121:9029
Carbapenem derivatives as antibiotics and intermediates thereof
Jung, Frederic Henri
Zeneca Ltd., UK; Zeneca Pharma S. A.
PCT Int. Appl., 44 pp.
CODEN: PIXXD2
Patent

INVENTOR(S):
PATENT ASSIGNEE(S):
SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA?	ENT	NO.			KIN	D	DATE			APPL	I CAT	ION	NO.		D.	ATE		
						-									-			
WO	9319	070			A1		1993	0930		WO 1	993-	GB60	3		1	9930	324	
	W:	AT,	AU,	BB,	BG,	BR,	CA,	CH,	CZ,	DE,	DK,	ES,	FI,	GB,	HU,	JP,	ΚP,	
		KZ,	LK,	LU,	MG,	NL,	NO,	PL,	RO									
	RW:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	
		BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	ML								
2A	9301	611			А		1993	0927		ZA 1	993-	1611			1	9930	305	
IL	1051	35			A1		2000	0131		IL 1	993-	1051	35		1	9930	323	
ΑU	9337	636			A1		1993	1021		AU 1	993-	3763	6		1	9930	324	
ΑU	6629	72			B2		1995	0921										
ΕP	5866	63			A1		1994	0316		EP I	993-	9067	40		1	9930	324	
£Ρ	5866	63			B1		1999	0929										
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IE,	IT,	LI,	LU,	MC,	NL,	PT,	SI
нυ	6571	3			A2		1994	072B		HU 1	993-	3304			1	9930	324	

(Continued) ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

CM 2

CRN 7087-68-5 CMF C8 H19 N

155481-36-0 HCAPLUS
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-{{[4-[(2-propenyloxy)carbonyl]-2-thienyl]amino[carbonyl]-, (4-nitrophenyl)methyleater, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

155481-37-1 HCAPLUS
1-Azabicyclo(3.2.0)hpt-2-ene-2-carboxylic acid, 3-[[5-[[(3-carboxy-4,5,6,7-tersphydrobenzo|b]thien-2-yl)amino|carbonyl|-1-[[(4-nitrophenyl|methoxy|carbonyl|-3-pyrrolidinyl]thio|-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 2-(2-propenyl) ester, (4R-[3(3S*,5S*),4a,5ß,6.be ta.(R*)])- [9CI] (CA INDEX NAME)

L8 ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) Absolute stereochemistry.

RN 155481-38-2 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[(3-carboxy-4,5,6,7-tetrahydrobenzo(bl)thien-z-yl)amino[carbonyl]-, 1-[(4-nitrophenyl)methyl]
ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 155481-40-6 HCAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[5-[[(3-carboxy-4-methyl-2-thienyl]amino]carbonyl]-1-[[(4-nitrophenyl]methoxy]carbonyl]-3-pyrrolidinyl]thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 2-(2-propenyl) eater, [4R-[3(35',58'),4a,5B,6B[R*]]-, compd. with N-ethyl-N-(1-methylethyl)-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CRN 155481-39-3 CMF C32 H34 N4 O11 S2

Absolute stereochemistry.

LB ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 155481-43-9 HCAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-(1-hydroxyethyl)-4-methyl-3-[[1-[(4-nitrophenyl)methoxy]carbonyl]-5-[[[5-[(2-propenyloxy)carbonyl]-2-thienyl]amino]carbonyl]-3-pyrrolidinyl]thio]-7-oxo-, (4-nitrophenyl)methyl ester, [4R-[3(35*,55*),4a,5β,6β(R*)])- [9C1] (CA INDEX NAME)

Absolute stereochemistry.

PAGE 2-A

RN 155481-44-0 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-mercapto-2-[[[5-[(2-propenyloxy)carbonyl]-2-thienyl]amino]carbonyl]-, (4-nitrophenyl)methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CM 2 CRN 7087-68-5 CMF C8 H19 N

Et | | i-Pr- N-Pr-

RN 155481-41-7 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-{acetylthio}-2-[[[3-(ethoxycarbonyl)-4-methyl-2-thienyl],amino]carbonyl]-, (4-nitrophenyl)methyl ester, (2S-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 155481-42-8 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 2-[[{3-carboxy-4-methyl-2-thienyl}amino[carbonyl]-4-mercapto-, 1-[(4-nitrophenyl)methyl] ester, (2S-cis)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 155481-45-1 HCAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[5-[[(5-carboxy-3-hydroxy-2-thienyl)amino]carbonyl]-1-[[[4-nitrophenyl]methoxy]carbonyl]-3-pyrrolidinyl]thio]-6-[1-hydroxyethyl)-4-methyl-7-oxo-, monosodium salt, [4R-[3(48-),5-),4a,5p,68[x+y]]-[9C] (CA INDEX NAME)

RN 155481-51-9 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[[3-(1,1-dimethylethoxy)-5-([1,1-dimethylethoxy)carbonyl]-2-thienyl]amino[carbonyl]-,
(4-nitrophenyl)methyl ester, (25-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

155481-52-0 HCAPLUS
1-Pyrrolidinecarboxylic acid, 2-[[[5-carboxy-3-hydroxy-2-thienyl]amino]carbonyl]-4-mercapto-, 1-[(4-nitrophenyl)methyl] ester, (2S-cis)- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

155481-53-1 HCAPLUS
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[5-[[(5-carboxy-3-hydroxy-2-thienyl]mino]carbonyl]-1-[[(4-nitrophenyl]methoxy]carbonyl]-3-pyrrolidinyl]thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 2-(2-propenyl) ester, {4R-[3(35*,5S*), 4u,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 28 May 1994

Title compds. [I; R1 = 1-hydroxyethyl, 1-fluoroethyl, hydroxymethyl; R2, R3 = H, alkyl; R4 = Q1-Q3; Z = carboxy, sulfonic acid, sulfinic acid, phenylsulfonylcarbamoyl, alkoxycarbamoyl, alkanesulfonamido, cyanocarbamoyl, tetrazol-5-yl, 3-hydroxyisoxazol-4-yl, benzamidosulfonyl, etc.] were prepared Thus, (ZS,4S)-1-(4-nitrobenzyloxycarbonyl)-2-(3-sulfophenylcarbamoyl)pyrrolidin-4-ylthioacetate dilaporpoylethylamine salt (preparation given) was asponified with 1N NaOH and the resulting thiol was stirred with 4-nitrobenzyl (IR,5K,6S,8H)-6-(1-hydroxyethyl)-1-methyl-2-diphenylphosphoryloxycarbapenem-3-carboxylate (preparation given) in DMF aining

stirred with 4-nitrobenzyl (1R, SR, 6S, 8R)-6-(1-hydroxyethyl)-1-methyl-2-diphenylphosphoryloxycarbapenem-3-carboxylate (preparation given) in DMF containing diisopropylethylamine and Bu3P to give a coupling product which was hydrogenated in EtOAc/H2O/EtOH containing KHCO3 to give (1S, 5S, 6S, 8R, 2'S, 4'S)-2-[2-(3-sulfophenylcarbamoyl)pyrrolidin-4-ythio]-6-(1-hydroxyethyl)-1-methylcarbapenem-3-carboxylic acid dipotassium salt. This showed MIC's of 0.125 and 0.015 µg/mL against Staphylococcus aureus Oxford and Escherichia coli DCO, resp.

ACCESSION NUMBER: 1594:265929 HCAPLUS
DOCUMENT NUMBER: 120:265929 HCAPLUS
TITLE: Preparation of (carbamoylpyrrolidinylthio)carbapenems as antibiotics
INVENTOR(S): Jung, Frederic Henri; Bertrandie, Alain Michel; Galt, Ronald Hilson Begg
PATENT ASSIGNEE(S): Zeneca Ltd., UK; Zeneca-Pharma Eur. Pat. Appl., 28 pp.

DOCUMENT TYPE: Patent EPXXDW
DOCUMENT TYPE: Patent English
English ACC. NUM. COUNT: 1
PATENT INFORMATION:

PAT	ENT NO.			KIN	•	DATE	:	AP	PLICA	TION	NO.		DAT	E	
	562855 562855			Al Bl	•		0929		1993	-3022	96		199	30325	
	R: AT,	BE.	CH.		DK.			GB, G	R. IE	. іт.	LI.	LU.	MC. N	L. PT.	SE
CA	2091309			AA			0927		1993					30309	
AT	179978			E		1999	0515	AT	1993	-3022	96		199	30325	
ES	2133358			T3		1999	0916	ES	1993	-3022	96		199	30325	
JP	06025244			A2		1994	0201	JP	1993	-6807	6		199	30326	
US	5571805			A		1996	1105	US	1994	-3023	94		199	40908	
PRIORITY	APPLN.	INFO.	. :					EP	1992	-4008	1 37	F	199	20326	
								EP	1992	-4008	39	F	199	20326	

Page 3630/08/2005

ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

 $\label{local-problem} $$15549-48-7$$$ HCAPLUS $$1-Azabicyclo[3.2.0]$$ hept-2-ene-2-carboxylic acid, $$3-[[5-[[(5-carboxy-3-hydroxy-2-thienyl)amino]-acid-1-[[(4-nitrophenyl)methoxy]carbonyl]-3-pyrrolidinyl|thio|-6-[1-hydroxyethyl]-4-methyl-7-oxo-, $$[4R-[3(3S*,5S*),4\alpha,5\alpha,6\beta(R^*)]]-$$ (CA INDEX NAME)$

Absolute stereochemistry.

ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS ON STN EP 1992-402700 US 1993-37171 (Continued) A 19921002 B1 19930326

OTHER SOURCE(S): MARPAT 120:269929
IT 154308-96-9F 154308-97-9F 154308-88-0P
154308-98-1F 154308-90-4F 154308-91-5F
154308-93-7F 154309-01-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for antibacterial)
RN 154308-86-8 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-([[5-(2-propenyloxy)carbonyl]-2-thienyl]amino)carbonyl]-, (4-nitrophenyl)methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

154308-87-9 HCAPLUS
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[(5-carboxy-2-thienyl)amino]carbonyl)-, 1-[(4-nitrophenyl)methyl] ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

154308-88-0 HCAPLUS
1-Pyrrolidinecerboxylic acid, 4-(acetylthio)-2-[[[5f((methylaulfonyl)amino)carbonyl]-2-thienyl]amino]carbonyl]-,
(4-nitrophenyl)methyl ester, (25-cis)- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

154308-89-1 HCAPLUS
1-Pyrrolidinecarboxylic acid, 4-mercapto-2-[[[5-[[(methylaulfonyl]maino]carbonyl]-,
(4-nitrophenyl)methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

 $\label{eq:continuous} $$1-Azabicyclo[3,2,0]$ pet-2-ene-2-carboxylic acid, $6-(1-hydroxyethy1)-4-methyl-3-[5-[[5-[[6-([methylsulfony1]amino]carbony1]-2-thienyl]amino]carbony1]-1-[[(4-nitropheny1)methoxy]carbony1]-3-pyrrolidinyl]thio]-7-oxo-, $(4-nitropheny1)methyl ester, $[4R-[3(3S^*,5S^*),4\alpha,5\beta,6\beta(R^*)]]-$(9CI)$ (CA INDEX NAME)$

Absolute stereochemistry.

ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN CM $\,^{1}$ (Continued)

CRN 154308-92-6 CMF C36 H33 N7 O12 S2

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

CM 2 CRN 7087-68-5 CMF C8 H19 N

154309-01-0 HCAPLUS
1-Pyrrolidinecarboxylic acid, 2-[[[5-[(cyanoamino]carbonyl]-2-thienyl]amino]carbonyl]-4-mercapto-, (4-nitrophenyl)methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

154308-91-5 HCAPLUS
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[[5-[(cyanoamino)carbonyl]-z-thienyl]mino]carbonyl]-, (4-nitrophenyl)methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

154308-93-7 HCAPLUS
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[5-[[5-[[5-[(cyanoamino)carbonyl]-2-thienyl]amino]carbonyl]-1-[[[4-nitrophenyl]methoxy]carbonyl]-3-pyrrolidinyl]thio]-6-[1-hydroxyethyl]-4-methyl-7-oxo-, (4-nitrophenyl)methyl ester, [4R-[3]35*,55*, [4x,5]5, [6](*)]]-, compd. with N-ethyl-N-(1-methylethyl)-2-propanamine [1:1] (9CI) (CA INDEX NAME)

L8 ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 05 Mar 1994

R1R2NA (CH2) nX1 CONH (CH2) 2C: NHNH2

AB Title compds. I (n = 0-6: A = bond, acylyl, aromatic heterocyclyl: X1 = bond, NHCO, CONN: X2. X3 = CONH, NHCO: R1, R2 = oxtranomethyl, laubsticuted) C2-4 alkyl, C2-4 alkoxyhalo, R402SO wherein R4 = C1-4 alkyl, Ph: R1 = H, R2 = R3(CH2)mCO wherein R3 = halo, oxtranyl, methyloxtranyl, aztridinyl, cyclopropyl, (substituted) C2-6 alkenyl, etc.) useful as anticancer and antivirus agents (no data), are prepared 4-(R2N)C6H4N(HOCH2CH2)2 in MeOH was added to a C6H6 solution of 1-methyl-4-(R1, N-bis (2-hydroxyethyl) aminol pherzeneaminocarbonyl]pyrrole-2-carboxylate which was asponified to the free acid which was converted to bis (2-chlorocethyl derivative which in DMF was added to 1-methyl-4-(1-methyl-4-aminopyrrole-2-carboxamido)pyrrole-2-carboxamidopyrrole-2-c

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

												_		
PAT	ENT NO	•		KIN	D DATE		AP	PLICAT	TON	NO.		D	ATE	
			-									-		
WO	931373	9		A2	1993	0722	WO	1993-	EP2			1	9930	104
WO	931373	9		A3	1993	1125								
	RW: A	T, BE	CH,	DĒ,	DK, ES,	FR, G	B, G	R, IE,	IT,	LU,	MC,	NL,	PT,	SÉ,
	В	F, BJ	CF,	CG,	CI, CM,	GA, G	N, M	L, MR,	SN,	TD,	TG			
AU	933347	8		A1	1993	0803	AU	1993-	3347	3		1	9930	104
EP	623023			Al	1994	1109	EP	1993-	9021	41		1	9930	104
	R: D	E, ES,	FR,	GB										
PRIORITY	APPLN	. INFO	o.:				IT	1992-	MI21			A 1	9920	110
							WO	1993-	EP2			A 1	9930	104

OTHER SOURCE(S): MARPAT 120:107751 150691-25-1P 150691-26-2P 150691-27-3P

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A - cн₂- сн₂с1 СH2-СH2С1

150691-27-3 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N2-(3-amino-3-iminopropyl)-N4-[4-[[4-[[4-[[14-[[1512-chloroethyl]amino]-2-thienyl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl|carbonyl]amino]-1-methyl-1H-pyrrol-2-yl|carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-, monohydrochloride (9C1) (CA INDEX NAME)

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS ON STN 150691-28-49 150691-29-59 150691-30-89 150691-33-19 150691-34-29 150691-35-39 150691-36-4P 150691-40-0P

130691-35-19 150691-36-4P 150691-40-0P
RE: SPN (Synthetic preparation): PREP (Preparation)
 (prepn. of, as anticancer and antivirus agent)
150691-25-1 HCAPLUS
1H-Pyrrola-2,4-dicarboxamide, N2-{5-[[[5-[[(3-amino-3-iminopropy])amino|carbonyl]-1-methyl-1H-pyrrol-3-yl]carbonyl]amino]-1-methyl-1H-pyrrol-3-yl]carbonyl]-1-methyl-th-pyrrol-3-yl]oarbonyl]-1-methyl-monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A н₂N- с- сн₂- сн₂- NH

> PAGE 2-A сн₂-сн₂с3 сн₂- сн₂с1

150691-26-2 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N2-[5-[[{3-amino-3-iminopropyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-N4-[4-[[4-[bis{2-chloroethyl]amino]benzoyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-, monohydrochloride (9CI) {CA INDEX NAME}

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

 $\label{local-29-5} \begin{array}{ll} \text{HCAPLUS} \\ \text{3H-Pyrrole-2, 4-dicarboxamide, N2-(3-amino-3-iminopropyl)-N4-(4-[\{[4-(bis(2-chloroethyl)amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-1, monohydrochloride (9CI) (CA INDEX NAME) \\ \end{array}$

L8 ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued

● HCl

RN 150691-30-8 HCAPLUS
CN 1H-Pyrrole-2,4-dicarboxamide, N2-[5-[[(3-amino-3-iminopropy)]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-N4-[4-[bia(2-chloroethyl)amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-, monohydrochloride
(9CI) (CA INDEX NAME)

● HCl

RN 150691-31-9 HCAPLUS
CN 1H-Pyrrole-2,4-dicarboxamide, N2-(3-amino-3-iminopropyl)-N4-[4-[[(4-[bis(2-chloroethyl)amino]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-

L8 ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued

PAGE 2-A

HC1

RN 150691-34-2 HCAPLUS
CN 1H-Pyrrole-2, 4-dicarboxamide, N2-(3-amino-3-iminopropyl)-N4-[4-[[4[(cyclopropylcarbonyl)amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1methyl-1H-pyrrol-2-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 2-A

HC1

RN 150691-35-3 HCAPLUS
CN 1H-Pyrrole-2,4-dicarboxamide, N2-(3-amino-3-iminopropyl)-N4-[4-[([4-[(1-aziridinylcarbonyl)amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

L8 ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) pyrrol-2-yl)-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

RN 150691-33-1 HCAPLUS
CN HH-Pyrrole-2, 4-dicarboxamide, N2-(3-amino-3-iminopropyl)-1-methyl-N4-[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[1]-methyl-4-[1]-methyl-4-[1]-methyl-3])-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]-, monohydrochloride (9CI) (CA INDEX NAME)

L8 ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

Me

NH

C- CH2- CH2- NH- C

NH

NH

C= 0

NH

C= 0

PAGE 2-A

● HC1

N 150691-36-4 HCAPLUS
N 1H-Pyrrole-2,4-dicarboxamide, N2-{3-amino-3-iminopropyl}-N4-{4-{{|{4-{(2-chloro-1-oxo-2-propenyl}amino}-1-methyl-1H-pyrrol-2-yl}carbonyl}amino}-1-methyl-1H-pyrrol-2-yl}-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

• нс

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 1H-Pyrrole-2, 4-dicarboxamide, N2-15-[[(3-amino-3-iminopropyl)aminojcarboxyl]-1-methyl-1H-pyrrol-3-yl]-N4-[4-[4-[4-[4-[bis(2-chiotoethyl)amino]phenyl]-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-1, monohydrochloride (SCI) (CA INDEX NAME)

● HC1

ΙT

150691-42-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of anticancer and antivirus agents)
150691-42-2 HCAPLUS
H-Pyrrole-2-carboxamide, 4-amino-N-[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-,

L8 ANSWER 29 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

Entered STN: 08 Jan 1994

High resolution proton NRM techniques have been used to study the interaction
between the self-complementary Dickerson dodecamer d(GGGGAATTCGCG)2 and
two distamycin namlogs containing a retroinverted amide bond. The results
indicated that both analogs, although binding the Dickerson dodecamer less
strongly than distamycin, span the central AATT segment in the minor
groove in a similar fashion.

ACCESSION NUMBER: 1994:2947 HCAPLUS
DOCUMENT NUMBER: 1994:2947 PROPERTY NUMBER: 1994:2947

TITLE: PROPERTY NUMBER: 1994:2947

PROPERTY NUMBER: 1994:2947

PROPERTY NUMBER: 1994:2947

DOCUMENT NUMBER: TITLE:

120:2947
Proton NMR studies of the interactions of two
distamycin analogs with the dodecamer d(CGCCAATTCGCG)2
Rosaria Conte, Maria; Fattorusso, Ernesto;
Gomez-Paloma, Luigi; Mayol, Luciano
Dip. Chim. Sostanze Nat., Univ. Napoli Federico,
Naples, I-80131, Italy
Bioorganic & Medicinal Chemistry Letters (1992),
2(10), 129-304
CODEN: BMCLE8; ISSN: 0960-894X AUTHOR (S):

CORPORATE SOURCE:

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN monohydrochloride (9CI) (CA INDEX NAME) (Continued)

● HC1

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 02 Oct 1993

Derivatives of "-amino-1-methyl-3-pyrrolecarboxamad as angiogenesis inhibitors
Mongelli, Nicola: Biasoli, Giovanni; Paio, Alfredo;
Mariani, Mariangela
Farmitalia Carlo Erba S.r.l., Italy
Brit. UK Pat. Appl., 43 pp.
CODEN: BAXXDU INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent English

PATENT NO. KIND DATE APPLICATION NO. DATE

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (9CI) (CA INDEX NAME) (Continued)

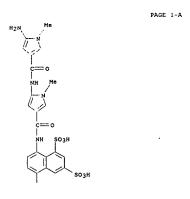
149594-72-9P 149594-73-0P

149594-72-99 149594-73-0P
RE: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reaction of in synthesis of angiogenesis inhibitor)
149594-72-9 HCAPLUS
1,3,5-Naphthalenetrisulfonic acid, 8-[[[5-[[[5-amino-1-methyl-1H-pyrrol-3-yl]carbonyl]amino]-1-methyl-1H-pyrrol-3-yl]carbonyl[amino]-1-methyl-1H-pyrrol-3-yl]carbonyl[amino]-1-methyl-1H-pyrrol-3-yl]ca

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

149594-76-3P 149621-63-6P 149621-70-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as angiogenesis inhibitor)
149594-76-3 HCAPLUS
1,3-Naphthalenedisulfonic acid, 7,7'-(carbonylbis(imino(1-methyl-1H-pyrrole-2,4-diyl)carbonyllmino(1-methyl-1H-pyrrole-2,4-diyl)carbonyllmino))bis-, tetrapotassium salt (9CI) (CA INDEX NAME)

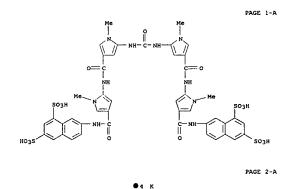
L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)



PAGE 2-A

149594-73-0 HCAPLUS
1,3,5-Naphthalenetrisulfonic acid, 8-[[[1-methyl-5-[[(1-methyl-5-nitro-lH-pyrrol-3-yl]carbonyl]amino]-lH-pyrrol-3-yl]carbonyl]amino]-, trisodium salt (SCI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)



149621-63-6 HCAPLUS
1H-Pyrrole-3-carboxamide, 5,5'-(carbonyldiimino)bis[N-[4-[[8-(dimethylamino)-1-naphthalenyl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-[9CI) (CA INDEX NAME)

149621-70-5 HCAPLUS
1,3,5-Naphthalenetrisulfonic acid, 8,8'-[carbonylbis{imino(1-methyl-lH-pyrrole-2,4-diyl)carbonylimino(1-methyl-lH-pyrrole-2,4-

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN diyl)carbonylimino]]bis- (9CI) (CA INDEX NAME) (Continued)

PAGE 2-A 503H

149594-70-7P
RL: SFN (Synthetic preparation): PREP (Preparation)
(preparation of, in synthesis of angiogenesis inhibitor)
149594-70-7 HCAPLUS
1H-Pyrrole-3-carboxamide, 5-amino-N-[4-[[8-(dimethylamino)-1-naphthalenyl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl}-1-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

●6 Na

149594-77-4
RL: RCT (Reactant): RACT (Reactant or reagent)
(reaction of, in synthesis of angiogenesis inhibitor)
149594-77-4
HCAPLUS
1,3-Naphthalenediaulfonic acid, 7-[[5-[[5-mino-1-methyl-1H-pyrrol-3-yl]carbonyl]amino]-1-methyl-1H-pyrrol-3-yl]carbonyl]amino]-1-methyl-1H-pyrrol-3-yl]carbonyl]amino]-,
monohydrochloride (9CI) (CA INDEX NAME)

• HC1

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ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

149594-71-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, protonation, and formulation of, as angiogenesis inhibitor)
149594-71-8 HCAPLUS
1,3,5-Naphthalenetrisulfonic acid, 8,8'-[carbonylbis[imino{1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino[]bis-, hexasodium salt (9CI) (CA INDEX NAME)

149621-72-7 149621-73-8 149621-74-9
149621-75-0 149621-76-1 149621-77-2
1496221-78-3 149621-96-1 149621-80-7
149621-81-1 149621-82-9 149621-80-7
149621-81-1 149621-85-2 149621-80-3
149621-81-1 149621-85-2 149621-86-3
149621-87-4
RL: RCT (Reactant): RACT (Reactant or reagent)
(use of, as angiogenesis inhibitor)
149621-72-7 HCAPLUS
1H-Pyrrole-3-carboxamide, 5,5'-(carbonyldiimino)bis[N-[4-([(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1

PAGE 1-A

PAGE 2-B

— с— NH2 || NH

149621-73-8 HCAPLUS Carbonimidic dihydrazide, 2,2'-bis[4-[[[4-[[[4-[[(3-amino-3-

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) iminopropyl)amino|carbonyl]-1-methyl-1H-pyrrol-2-yl]amino|carbonyl]-1-methyl-1H-pyrrol-2-yl]amino|carbonyl]-1-methyl-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 149621-74-9 HCAPLUS
CN 1-Naphthalenesulfonic acid, 4,4'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino]bis-(9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

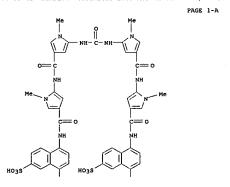
RN 149621-76-1 HCAPLUS
CN 1,3-Naphthalenedisulfonic acid, 8,8'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino]]bis- (9CI) (CA INDEX NAME)

RN 149621-77-2 HCAPLUS
CN 1.7-Naphthalenedisulfonic acid, 4.4'-[carbonylbis|imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino||bis- (9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 149621-75-0 HCAPLUS
CN 1-Naphthalenesulfonic acid, 8,8'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino)]bis-(9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)



PAGE 2-A | | | SO3H SO3H

IN 149621-78-3 HCAPLUS 1.5-Naphthalenedisulfonic acid, 4,4'-[carbonylbis[imino(1-methyl-lH-pyrrole-2,4-diyl)carbonylimino(1-methyl-lH-pyrrole-2,4-diyl)carbonylimino]]bis- (9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A PAGE 2-A

149621-79-4 HCAPLUS
1,3,6-Naphthalenetrisulfonic acid, 8,8'-[carbonylbis{imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino{1-methyl-1H-pyrrole-2,4-diyl)carbonylimino]]bis- (9CI) (CA INDEX NAME)

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

149621-81-8 HCAPLUS
1,3-Naphthalenedisulfonic acid, 6,6'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino]]bis-(9CI) (CA INDEX NAME)

149621-82-9 HCAPLUS
1,7-Maphthalenedisulfonic acid, 3,3'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino)]bis- (9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

149621-80-7 HCAPLUS
1,5-Maphthalenedisulfonic acid, 7,7'-(carbonylbis(imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino)]bis-(9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

149621-83-0 HCAPLUS
2,7-Maphthalenedisulfonic acid, 3,3'-[carbonylbis[imino(1-methyl-1H-pyrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrole-2,4-diyl)carbonylimino]}bis- (9CI) (CA INDEX NAME)

PAGE 1-A

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-B

− so₃H

RN 149621-84-1 HCAPLUS
CN 1,3,5-Naphthalenetrisulfonic acid, 7,7'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino]bis- (9CI) (CA INDEX NAME)

RN 149621-85-2 HCAPLUS
CN 1,3-Maphthalenedisulfonic acid, 7,7'-[carbonothioylbis[imino(1-methyl-1H-pyrrole-2,4-dtyl)carbonylimino[1-methyl-1H-pyrrole-2,4-dtyl)carbonylimino]bis- (9CI) (CA INDEX NAME)

LB ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-B

RN 149621~87-4 HCAPLUS
OF D-Glucose, 2,2'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4diyl](arbonylimino(1-methyl-1H-pyrrole-2,4-diyl)(arbonylimino)]bis(2-deoxy-,6,6'-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 149621-86-3 HCAPLUS

CN D-Glucose, 2,2'-|carbonylbis|imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino|}bis{2-deoxy-,6,6'-bis(hydrogen sulfate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HO3SO OH CHO OH NH ME OH NH ME OH ME ME

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-B

O CHO OH OPO 3H2

De Entered STN: 18 Sep 1993

AB Comparison of the DNA cleavage activity of man-designed bleomycins demonstrates that bleomycins are small enzymes comprised of the catalytic site and a binding site. The linker moiety is shown to be significant for DNA binding, and inversion of its stereochem, results in a dramatic decrease in the DNA-cleaving efficiency. It can be said that bleomycin possesses a switching device in the β-aminoalaninamide moiety to regulate the in vivo activity. One of the man-designed BLMs shows excellent cytotoxicity against Lizio.

ACCESSION NUMBER: 1993:508375 HCAPLUS

DOCUMENT NUMBER: 11991:508375 Man-designed bleomycins: Significance of the binding sites as enzyme models, of the stereochemistry of the linker moiety, and of a switching device in the β-aminoalaninamide moiety

AUTHOR(S): Ohno, Massji

CORPORATE SOURCE: SOURCE:

AUTHOR (S):

N-aminoalaninamide molety
Ohno, Masaji
Fac. Pharm. Sci., Univ. Tokyo, Tokyo, Japan
Proceedings of the Robert A. Welch Foundation
Conference on Chemical Research (1991), 35(Chem.
Front. Med.), 119-34
CODEN: PRAWAC: ISSN: 0557-1588

DOCUMENT TYPE:

149352-73-8

RL: RCT (Reactant); RACT (Reactant or reagent)

RL: RCT (Reactant); RACT (Reactant or reagent)
(deprotection of)
149352-73-8 HCAPLUS
Carbamic acid, (4-[15-[[[5-[[[5-[[[3-[dimethylamino)propyl]amino]carbonyl]1-methyl-1H-pycrol-2-yllamino]carbonyl]-1-methyl-1H-pycrol-2yllamino[carbonyl]-1-methyl-1H-pycrol-2-yllamino]-4-oxobutyl]-,
1,1-dimethylethyl ester (9C1) (CA INDEX NAME)

PAGE 1-B

149330-07-4P

149330-07-4P
REL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with distamycin)
149330-07-4 HCAPLUS
H-Pyrrole-2-carboxamide, 5-[[[5-[(4-amino-1-oxobutyl)amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-N-[5-[[[3-(dimethylamino)propyl]amino]carbonyl

L8 ANSWER 32 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

Entered STN: 07 Aug 1993
AB Nonintercalating DNA minor-groove binders may effectively inhibit the supercoiling activity of DNA gyrase (I) by influencing the enzyme recognition and cleavage site on DNA. For I from Streptomyces noursel, a wide range of inhibitory potency for different classes of ligands was observed This could be explained by a number of structural and binding factors of the ligands competing with I on the target site of DNA, the mechanism of which is different from the classical I inhibitors.

ACCESSION NUMBER: 1993:443973 HCAPLUS

DOCUMENT NUMBER: 119:43973

Minor-groove binders are inhibitors of the catalytic

DOCUMENT NUMBER: TITLE: 119:43973
Minor-groove binders are inhibitors of the catalytic activity of DNA gyrases
Stoerl, K.; Stoerl, J.; Zimmer, Ch.; Lown, J. W.
Dep. Mol. Biol., Inst. Mol. Biol., Univ. Jena, Jena, Germany
FEBS Letters (1993), 317(1-2), 157-62
CODEN: FEBLAL; ISSN: 0014-5793
Journal
Fendish

AUTHOR(S): CORPORATE SOURCE:

SOURCE:

DOCUMENT TYPE:

DOUGHET TIPE: Southal
LANGUAGE: English

IT 148504-19-2 148504-20-5 148504-21-6
RL: BIOL (Biological study)
(DNA gyrase of Streptomyces noursei inhibition by, mechanism of)

RN 148504-19-2 HcAPPLUS

CN Heptanediamide, N,N'-bis[5-[[[5-{[(3-amino-3-iminopropyl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]- (9CI) (CA

PAGE 1-B

148504-20-5 HCAPLUS
Octanediamide, N,N'-bis[5-[[[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

ANSWER 31 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)]-1-methyl-1H-pyrrol-2-yl)-1-methyl- (9CI) (CA INDEX NAME)

PAGE 1-B

- (CH2) 3 - NH2

PAGE 1-B

148504-21-6 HCAPLUS
Decanediamide, N,N'-bis[5-[[5-[[3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

L8 ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 04 Oct 1992

AB HXIZXZZX3ZCONHCHZCHZC(:NH)NHZ (X1, X2, X3 = CONH or NHCO the case wherein X1 = X2 = X3 = CONH being excluded; Z = 1-methyl-2,4-pyrrolylene throughout) were prepared as antiviral and antitumor agents (no data). Thus, NOZCZCOZHE and OZNZCOM3 (preparation each given) were heated with Et3N and the product converted in 3 steps to OZNZHCOZCONHCHZCHZC(:NH)NHZ which was hydrogenated and the product condensed with HCONHZCOZH (preparation given) to give NCONHZCHCCONHCHZC(:NH)NHZ.

ACCESSION NUMBER: 1992:330993 HCAPLUS

DOCUMENT NUMBER: 1992:330993 HCAPLUS

Preparation of distamycin analogs as antiviral

117:130993
Preparation of distamycin analogs as antiviral antitumor agents
Animati, Pablo; Arcamone, Federico; Lombardi, Paolo; Rossi, Cristina
Menarini, A., Industrie Farmaceutiche Riunite S.r.l., Italy; Bristol-Myers Squibb S.p.A.
PCT Int. Appl., 39 pp.
CODEN: PIXXD2
Patent
English 1
1

INVENTOR (S):

PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:			
PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 9209574	A2 19920611	WO 1991-EP2220	19911120
WO 9209574	A3 19920806		
W: AU, BB, BG,	BR, CA, CS, FI,	HU, JP, KP, KR, LK,	MC, MG, MN, MW,
NO, PL, RO,	SD. SU. US		
RW: AT, BE, BF,	BJ, CF, CG, CH,	CI, CM, DE, DK, ES,	FR, GA, GB, GN,
GR, IT, LU,	ML, MR, NL, SE,	SN, TD, TG	
AU 9189178	A1 19920625	AU 1991-89178	19911120
PRIORITY APPLN. INFO.:		IT 1990-22154	A 19901122
		WO 1991-EP2220	A 19911120
OTHER SOURCE(S):	MARPAT 117:1309	93	

143158-63-8P 143158-64-9P 143158-65-0P 143363-83-1P

143363-83-19
REP (Preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction of, in preparation of antiviral and antitumor

agents;
RN 143158-63-8 HCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 1-methyl-4-[[(1-methyl-4-nitro-1H-pyrrol-2-yl)amino]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

143158-59-2 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N4-[4-[{[4-{aminocarbonyl}-1-methyl-1H-pyrrol-2-yl]-N2-(3-amino-3-iminopropyl)-1-methyl- (9CI) (CA INDEX NAME)

143158-60-5 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N2-[5-[[(3-amino-3-iminopropy]) amino|carbonyl]-1-methyl-1H-pyrrol-3-yl]-N4-[4-(formylamino)-1-methyl-1H-pyrrol-2-yl]-1-methyl- (9CI) (CA INDEX NAME)

ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 1H-Pytrole-2-carboxylic acid, 1-methyl-4-[[(1-methyl-4-nitro-1H-pytrol-2-ylamino]carbonyl]- (9CI) (CA INDEX NAME)

143158-65-0 HCAPLUS
1H-Pyrrole-2,4-dicarboxamide, N2-(2-cyanoethyl)-1-methyl-N4-(1-methyl-4-nitro-1H-pyrrol-2-yl)- (9CI) (CA INDEX NAME)

143363-83-1 HCAPLUS
1H-Pyrrole-2,4-dicarboxamide, N2-(3-amino-3-iminopropyl)-1-methyl-N4-(1-methyl-4-nitro-1H-pyrrol-2-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

143158-61-6 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N4-[4-(aminocarbonyl)-1-methyl-1H-pyrrol-2-yl]-N2-[5-[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl- (9C1) (CA INDEX NAME)

143158-66-1 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N2-(3-amino-3-iminopropyl)-N4-[4-[[4-(formylamino)-1-methyl-1H-pyrrol-2-yl]amino]carbonyl}-1-methyl-1H-pyrrol-2-yl]-1-methyl-(9CI) (CA INDEX NAME)

ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

143158-67-2 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N4-[4-[[[4-{aminocarbonyl}]-1-methyl-1H-pyrrol-2-yl]amino]-carbonyl]-1-methyl-1H-pyrrol-2-yl]-N2-(3-amino-3-iminopropyl)-1-methyl- (9CI) (CA INDEX NAME)

ANSWER 35 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 17 Apr 1992

AB Title compds. [I; A = (un) substituted N-containing heterocyclylenediyl; Q = BN-RBR9R10, heterocyclyl, heterocyclylalkyl; B = alkylene alkylidene; R1 = H, Mer R2 = H, alkyl; NQR2 = heterocyclyl group Q1; R3 = H, neg. charge; R6 = (un) substituted alkyl; R7-R10 = alkenyl, alkynyl, (un) substituted alkyl; m, n = 0-2] were prepared Thus, (2S, 4S)-4-(4-methoxybenzylthio)-2-pyrrolidinecarboxylic acid was N-protected and the product amidated with N-methylpiperazine to give, after hydrolysis, (2S, 4S)-4-mercapto-2-(4-methyl-1-piperazinylcarbonyl)-1-(4-hitrobenzyloxycarbonyl)pyrrolidine. The latter was stirred 5 h at .apprx.0° with 4-nitrobenzyl [Q1R, SR, 6S)-6-([R]N-hydroxymethyl]-1-methyl-2-coxo-1-methyl-2-coxo-1-carbapenem-3-carboxylate which had been treated with Ph2P(0)C1 and the product treated with F8C20Me followed by catalytic hydrogenolysis to give title compound (1R, SS, 6S)-II which had MIC of SO.01 (no units given) against Staphylococcus aureus 209P and Escherichia coli NIHJ. I are resistant to dehydropeptidase I and B-lactamase.

ACCESSION NUMBER: 1992:151432 MCAPLUS

COUNDENT NUMBER: 1992:151432 MCAPLUS

Carbapenems and analogs as antibiotics

116:151432
Preparation of { (piperaziniocarbonyl) pyrrolidinylthio} carbapenems and analogs as antibiotics
Kawamoto, Isao: Miyauchi, Masao: Nakayama, Eiji: Endo, Rokoro: Ohya, Satoshi: Utsui, Yukio
Sankyo Co., Ltd., Japan
Eur. Pat. Appl., 117 pp.
CODEN: EPXXDW
Patent INVENTOR (S):

PATENT ASSIGNEE (S):

SOURCE:

DOCUMENT TYPE:

LANGUAGE : FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
	A1 19910828 DE, DK, ES, FR,	GB, GR, IT, LI, LU, NL,	
JP 04211083	A2 19920803		19910221
CA 2036941	AA 19910824		19910222
FI 9100860	A 19910824	FI 1991-860	19910222

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L8 ANSWER 34 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN
EDE Entered STN: 23 Aug 1992
B Various aliphatic N-acyl derivs. and an N-phthalidyl derivative of the model compound N-benzyloxycarbonyl-glycyl-L-prolineamide (2-Gly-ProNH2) were synthesized to assess their suitability as prodrug forms for the C-terminal prolineamide residue occurring in several peptides (e.g. TRH) with the aim of protecting the peptide against prolyl endopeptidase in the gut prior to absorption. Whereas Z-Gly-ProNH2 was rapidly hydrolyzed in a rabbit gut homogenate, used as a source of prolyl endopeptidase, the N-acyl derivs. were found to afford protection by a factor of 1.5-6. The stability of the N-acyl derivs. in the gut homogenate decreased with increasing chain length within the acyl group. The N-phthalidyl derivative, on the other hand, degraded even faster than the parent compound The derivs. were all converted quant. into the parent peptide in human plasma solns, via hydrolysis catalyzed by non-specific plasma esterases. The results suggest that by appropriate N-acylation it may be feasible to improve the stability of a C-terminal prolineamide moiety toward prolyl endopeptidase. The combination of increased stability in the intestine and higher lipophilicity of the N-acyl prodrugs might render it possible to improve the delivery characteristics of peptides containing a C-terminal prolineamide moiety.

ACCESSION NUMBER: 1992:476326 HCAPLUS
DOCUMENT NUMBER: 17:76326
TITLE: Prodrugs of peptides. 17. Bioreversible derivatization of the C-terminal prolineamide residue in peptides to afford protection against prolyl endopeptidase

Moess, Judi's Bundgaard, Hans
CORPORATE SOURCE: Den.

SOURCE: International Journal of Pharmaceutics (1992), 82(1-2), 91-7

SOURCE:

Den.
International Journal of Pharmaceutics (1992),
82(1-2), 91-7
CODEN: JJPHDE; ISSN: 0378-5173
Journal

DOCUMENT TYPE: LANGUAGE: IT 142755-61-1P

142755-61-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and hydrolysis of, for protection against prolyl endopeptidase)
142755-61-1 HCAPLUS
L-Prolinamide, N-[(phenylmethoxy|carbonyl]glycyl-N-(1,3-dihydro-3-oxo-1-isobenzofuranyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8	ANSWER 35 C	F 41	HCAPLUS	COPYRIGHT	2005	ACS on STN	(Continued)
	FI 96863		В	19960531			
	FI 96863		С	19960910			
	NO 9100723		A	19910826	NO	1991-723	19910222
	NO 178498		В	19960102			
	NO 178498		С	19960410			
	AU 9171322		A1	19910829	AU	1991-71322	19910222
	AU 646012		B2	19940203			
	HU 58100		A2	19920128	HU	1991-620	19910225
	ZA 9101344		A	19921125	ZA	1991-1344	19910225
	CZ 289263		В6	20011212	cz	1991-483	19910225
	US 5310735		A	19940510	US	1992-938483	19920831
	RU 2059639		Cl	19960510	RU	1993-4744	19930315
	US 5420119		A	19950530	US	1993-143996	19931027
PRI	ORITY APPLN.	INFO.:			JP	1990-42796	A 19900223
					JP	1990-212283	A 19900810
					US	1991-658975	B1 19910221
					US	1992-938483	A3 19920831
						1003 60017	81 10020612

OTHER SOURCE(S): MARPAT 116:151432 138508-14-2P

138508-14-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction of, in preparation of antibiotics) 138508-14-2 HCAPLUS
138508-14-2 HCAPLUS
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-(1-hydroxyethyl)-4-methyl-3-[[5-([(1-methyl-2-pyrrolidinyl)]molocarbonyl]-1-[[(4-nitrophenyl)methoxylogratbonyl]-3-pyrrolidinyl]thio]-7-oxo-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

(Continued)

L8 ANSWER 36 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 05 Oct 1991

AB Bifunctional mols., e.g. tri, tetra-, penta-, and hexa-Nmethylpyrrolecarboxamide-EDTA, bis(EDTA-distamycin), etc., are prepared by
reacting a DNA intercalator (p-carboxymethidium, etc.) or DNA groove
binder (netropsin, distamycin, etc.) with 1,3-diaminopropane followed by
condensation with EDTA. These mols. are used for cleaving single- or
double-stranded DNA in the presence of Fe(II) and O with sequence
specificity which is either similar to or not available with naturally
occurring restriction enzymes. Thus, bis(EDTA-distamycin)phenoxazone was
prepared by using 3-benzyloxy-4-methyl-2-nitrobenzoic acid and
4-nitro-tri-N-methylpyrrole-2-carboxylic acid as starting materials, and
showed 1005 cleavage of plasmid pBR322 DNA at 20.1 µM in the
presence of Fe(II), 0, and dithiothreitol.
ACCESSION NUMBER: 15:31393 HCAPLUS
DOCUMENT NUMBER: 15:31393

TITLE: Preparation of bifunctional molecules having a DNA
intercalator or DNA groove binder linked to EDTA for
cleaving double-stranded DNA
Dervan, Peter B., Hertzberg, Robert P.
California Institute of Technology, USA
U.S., 59 pp. Cont.-in-part of U.S. 4,665,184.
CODEN: USXXAM
POCCUMENT TYPE:
LANGUAGE: NUM COLDIT.

DOCUMENT TYPE: LANGUAGE: LANGUAGE: English FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4942227	А	19900717	US 1987-6442	19870123
US 4665184	Α	19870512	US 1986-860604	19860507
PRIORITY APPLN. INFO.:			US 1982-338327 E	32 19820111
			US 1983-540914 E	31 19831012
			US 1986-860604 A	19860507
			US 1982-338332 A	A2 19820111

OTHER SOURCE (S) MARPAT 115:131393

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and reaction of, in preparation of bifunctional mols. having a

intercalator or DNA groove binder linked to EDTA for specific DNA

ANSWER 37 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 08 Dec 1990

AB Title compds. I [R2 = H, alkyl, Cl, (un)substituted Ph, (un)substituted Ph(PhH2; R4 = N, 1 or 2 substituents such as alkyl, HO, alkoxy, halo in 4-, 5-, 6-, or 7 position; alk = (un)substituted o,=alkylene (CH2)n; n = 2-6; NB = N3, H2N, alkylamino, hydroxyalkylamino, morpholino, thiomorpholino, piperidino, pyretolidino, attaino, pyrrolidino, 1-piperazinyl, hexahydro-4H-1,4-diazepinyl, their oxides, etc.] or an acid addition salt thereof, useful as analgesics (no data) are prepared II (R = R3CZ, R3COCH:CH, R3CO; R3 = cyclohexyl, heterocycylphenyl, aminomethylphnyl, (un)substituted styryl, biphenyl, (un)substituted naphthyl, heterocycyl, etc.; C2 = CO, HONC; R1 = H, BNAlk, BNCHZCH(HOH)CH2) were also prepared and found to possess analgesic, antiinflammatory and antirheumatic activities. II [R = 3-(GN)C6H4CO; R1 = 2-morpholinoethyl; R2 = Me; R4 = H] in EtOAc and AcOH was reduced with H over Pt oxide to give 831 II (R = 3-(HZN)C6H4CO; R4 = morphoninoethyl; R2 = Me; R4 = H] (III). III, on oral administration, showed and EDSO in acetylcholine-induced abdominal constriction and antibradykinin test of 16 and 53 mg, resp., and on the rat paw flexion test 0.12i at 100 mg/kg.

ACCESSION NUMBER: 1990:611828 HCAPLUS

DOCUMENT NUMBER: 1990:611828 HCAPLUS

INVENTOR(S): Bell Malcolm R.

PATENT ASSIGNEE(S): Sterling Drug Inc., USA

CODE: CAXXA4

DOCUMENT TYPE: Patent

DOCUMENT TYPE: Patent

LANGUAGE: English

DOCUMENT TYPE: FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 1258070	A2	19890801	CA 1988-576124	19880830
US 4581354	А	19860408	US 1985-755239	19850715
CA 1246563	A1	19881213	CA 1985-488073	19850802
US 4634776	А	19870106	US 1985-810942	19851219
US 32761	E	19881004	US 1987-29302	19870323
CA 1255305	A2	19890606	CA 1988-576122	19880830
CA 1255316	A2	19890606	CA 1988-576123	19880830
CA 1255312	A2	19890606	CA 1988-576125	19880830
CA 1258069	A2	19890801	CA 1988-576121	19880830
US 4885295	A	19891205	US 1988-255305	19881011
FI 8903253	A	19890704	FI 1989-3253	19890704
FI 8903254	A	19890704	FI 1989-3254	19890704
FI 8903255	A	19890704	FI 1989-3255	19890704
FI 8903256	А	19890704	FI 1989-3256	19890704
FI 8903257	A	19890704	FI 1989-3257	19890704
US 4978664	A	19901218	US 1989-409913	19890920
NO 9003304	А	19860207	NO 1990-3304	19900725

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L8	ANSWER 37 OF 41	HCAPLUS	COPYRIGHT	2005 ACS on STN	(Continued)
	NO 9003305	A	19860207	NO 1990-3305	19900725
	NO 9003306	A	19860207	NO 1990-3306	19900725
	US 5013732	А	19910507	US 1990-559787	19900730
PRIC	RITY APPLN. INFO.:			US 1984-637931	A 19840806
				US 1985-755239	A 19850715
				CA 1985-488073	A3 19850802
				FI 1985-2973	A 19850801
				NO 1985-3066	A1 19850802
				US 1985-810942	A3 19851219
				US 1986-928335	A1 19861107
				US 1988-255305	A3 19881011
				US 1989-409913	A3 19890920
OTHE	R SOURCE(S):	CASRE	ACT 113:21	1828; MARPAT 113:21	1828

125019-12-7P 125019-12-TP
RE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); TRU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as analgesic, antiinflammatory, and antirheumatic) 125019-12-7 HCAPLUS HI-Indole-3-carboxamide, N-methyl-1-[1-methyl-2-(4-morpholinyl)ethyl]-N-1H-pyrrol-2-yl-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 38 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 21 Jan 1989 GI

AB The title compds. [I; Rl, R2 = H, Cl-6 alkyl, C3-7 cycloalkyl,
 (un)substituted heterocyclyl; X = H, Cl-4 alkyl, Cl-4 alkoxy, Cl-4
 alkylthio, Br, Cl, F; Y = X, C3-6 cycloalkyl, CF3, NO2, MeCO, EtCO, PrCO,
 PhCO, thenoyl; adjacent XY = OCH2O] were prepared as inflammation inhibitors
 and analgesics (no data). To a slurry of 13.3 g oxindole (2-indolinone)
 in PhMe was added 15.6 g ClSO2NCO and the mixture heated on a steam bath to
 give 1-{chlorosulfonyllcarbamoylloxindole which was heated in aqueous HOAc to
 give 11.48 g 1-carbamoyloxindole. The latter (1.0 g) and 1.28 g
 2,4-Cl2C6H3NCO were stirred at 1 h 0-5* in DMF containing EtJN,
 followed by addition of IN HCL and stirring 20 min. to give 290 mg I (R1 =
 2.4-Cl2C6H3NCO were stirred at 1 h 0-5* in DMF containing EtJN,
 followed by addition of IN HCL and stirring 20 min. to give 290 mg I (R1 =
 2.4-Cl2C6H3NCO were stirred at 1 h 0-5* in DMF containing EtJN,
 followed by addition of IN HCL and stirring 20 min. to give 290 mg I (R1 =
 2.4-Cl2C6H3NCO were stirred at 1 h 0-5* in DMF containing EtJN,
 followed by addition of IN HCL and stirring 20 min. to give 290 mg I (R1 =
 2.4-Cl2C6H3NCO were stirred at 1 h 0-5* in DMF containing EtJN,
 followed by addition of IN HCL and stirring 20 min. to give 290 mg I (R1 =
 2.4-Cl2C6H3NCO were stirred at 1 h 0-5* in DMF containing EtJN,
 followed by addition of IN HCL and stirring 20 min. to give 290 mg I (R1 =
 2.4-Cl2C6H3NCO were stirred at 1 h 0-5* in DMF containing EtJN,
 followed by addition of IN HCL and stirring 20 min. to give 290 mg I (R1 =
 2.4-Cl2C6H3NCO were stirred at 1 h 0-5* in DMF containing EtJN,
 followed by addition of IN HCL and stirring 20 min. to give 290 mg I (R1 =
 2.4-Cl2C6H3NCO were stirred at 1 h 0-5* in DMF containing EtJN,
 followed by addition of IN HCL and stirring 20 min. to give 290 mg I (R1 =
 2.4-Cl2C6H3NCO were stirred at 1 h 0-5* in DMF containing EtJN,
 followed by addition of IN HCL and stirring 20 min. to give 290 mg I (R1 =
 2.4-Cl2C6H3NCO were stirre

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT INFORMATION:

PRI

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4725616	A	19880216	US 1987-8105	19870120
ZA 8605019	Α	19880224	ZA 1986-5019	19860707
DD 251971	A5	19871202	DD 1986-292280	19860708
US 4791129	A	19881213	US 1987-118123	19871109
ORITY APPLN. INFO.:			US 1985-753200	A2 19850709
			US 1987-8105	A3 19870120

OTHER SOURCE(S): CASREACT 110:2372
IT 107315-25-3P 107315-36-6P 107315-56-0P 107315-80-0P CASREACT 110:23728; MARPAT 110:23728

IN 137-90-09

RE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antiinflammatory)
107315-25-3 HCAPLUS
1H-Indole-1,3-dicarboxamide, 2,3-dihydro-2-oxo-N3-2-thienyl- (9CI) (CA INDEX NAME)

(Continued) ANSWER 38 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ANSWER 38 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

107315-36-6 HCAPLUS 1H-Indole-1, 3-dicarboxamide, 5-chloro-2, 3-dihydro-2-oxo-N3-2-thienyl-(9CI) (CA INDEX NAME)

107315-56-0 RCAPLUS
1H-Indole-1,3-dicarboxamide, 2,3-dihydro-N1-(4-methoxyphenyl)-2-oxo-N3-2-thienyl- (9C1) (CA INDEX NAME)

107315-80-0 HCAPLUS

5H-1,3-Dioxolo(4,5-f)indole-5,7-disarboxamide, 6,7-dihydro-N5-(4-methoxyphenyl)-6-oxo-N7-2-thienyl- (9CI) (CA INDEX NAME)

ANSWER 39 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 15 May 1987

AB The title compds. [I; n = 0-4; R = NHR3 [R3 = CON(NO)R4 [R4 = C1-4 (halo)alkyl], CO(CR2)mR5 (R5 = halo, oxiranyl, methyloxiranyl, aziridinyl, cyclopropyl, moiety of alicyclic a, B-unsatd. Ketone or lactone:

m = 0-4], NR6R7 [R6, R7 = oxiranylmethyl, aziridinylmethyl, substituted
C2-4 alkyl; l of R6, R7 = H, the other as above], NO2, NH2, NHCHO; R1 = H,
C1-6 alkyl; R2 = substituted C1-6 alkyl] and their pharmaceutically
tolerable salts, useful as antiviral and antineoplastic agents, were
prepared by 6 methods, e.g. reaction of aminopyrrolecarboxamide II (q = 1-5)
with nitropyrrole III (Z = leaving group) to give I (R = NO2).
3-[1-Methyl-4-[1-methyl-4-aminopyrrole-2-carboxamido]pyrrole-2-carboxamido derivatives,
procedure for their preparation and services,
procedure for their preparation and services,

106:136157
Polly-4-aminopyrrole-2-carboxamide derivatives,
procedure for their preparation, and antiviral and
antineoplastic pharmaceuticals containing them
Arcamone, Federico: Mongelli, Nicola: Penco, Sergio
Farmitalia Carlo Etba S.p.A., Italy
Ger. Offen., 35 pp.
CODEN: GWXXBX
Patent INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3623880	A1	19870129	DE 1986-3623880	19860715
US 4766142	A	19880823	US 1985-783588	19851003
SE 8603098	A	19870117	SE 1986-3098	19860711
SE 468642	В	19930222		
SE 468642	c	19930617		

LB ANSWER 39 OF 41	HCAPLUS	COPYRIGHT	2005 ACS on STN	(Continued)
AT 8601888	А	19880415	AT 1986-1888	19860711
AT 387013	В	19881125		
AU 8660202	Al	19870122	AU 1986-60202	19860714
AU 587841	B2	19890831		
NL 8601837	А	19870216	NL 198€-1837	19860714
HU 43088	A2	19870928	HU 1986-2904	19860714
HU 205949	В	19920728		
ES 2000502	A6	19880301	ES 1986-290	19860714
IL 79402	Al	19910610	IL 1986-79402	19860714
BE 905110	Al	19870115	BE 1986-216924	19860715
DK 8603359	A	19870117	DK 1986-3359	19860715
NO 8602860	A	19870119	NO 1986-2860	19860715
NO 168826	В	19911230		
NO 168826	C	19920408		
FR 2585018	A1	19870123	FR 1986-10294	19860715
FR 2585018	B1	19890713		
ZA 8605263	A	19870325	ZA 1986-5263	19860715
JP 62077362	A2	19870409	JP 1986-164879	19860715
SU 1544185	A3	19900215	SU 1986-4027809	19860715
CH 674206	A	19900515	CH 1986-2820	19860715
CA 1285934	A1	19910709	CA 1986-513760	19860715
FI 8602959	A	19870117	FI 1986-2959	19860716
FI 83640	В	19910430		
FI 83640	С	19910812		
GB 2178036	A1	19870204	GB 1986-17292	19860716
GB 2178036	B2	19890816		
CN 86104787	А	19870218	CN 1986-104787	19860716
CN 1018825	В	19921028		
CS 276981	B6	19921118	CS 1986-5412	19860716
SU 1609445	A3	19901123	SU 1987-4203699	19871126
PRIORITY APPLN. INFO	.:		GB 1985-17922	A 19850716
			GB 1986-13594	A 19860604
IT 107580-36-9P				

107580-36-99
RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of, as antiviral and antineoplastic agent)
107580-36-9 HCAPLUS
1H-Pyrrole-2-carboxamide, N-[5-[[[5-[[3-(dimethylamino)propyl]amino]carbo
nyl]-1-methyl-1H-pyrrol-3-yllamino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1methyl-4-[[[1-methyl-4-[[(1-methyl-4-filtro-1H-pyrrol-2-yl)amino]carbonyl]1H-pyrrol-2-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

ANSWER 40 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 01 May 1987

AB The title compds. I [X = H, Br, Cl, F, Cl-4 alkyl, alkylthio, alkoxy, C3-6 cycloalkyl, NO2, CF3, C2-4 acyl, Bz, thenoyl: Y = H, Br, Cl, Cl-4 alkyl, alkoxy, alkylthio: optionally XY = 4,5-, 5,6-, 6,7-OCHZO: A = NHR2. R3, NHCOR3: Rl, R2 = H, Cl-6 alkyl, C3-7 cycloalkyl, heterocyclyl, (substituted)Ph; R3 = Cl-6 alkyl, Ph] and their salts, prepared by the reaction of the appropriate oxindole with R1NCO or R1NNI2, are useful as antinfiammatory and analgesic agents (no data). To l-carbamoyloxindole, and Et3N in DNF, was added 2,4-C12C6H3NCO to give after addition of 1N HCl I (X = Y = H; A = NHZ; R1 = 2,4-C12C6H3).

ACCESSION NUMBER: 1967:38254 HCAPLUS
DOCUMENT NUMBER: 1967:38254 HCAPLUS
DOCUMENT NUMBER: 1967:38254 HCAPLUS
DOCUMENT NUMBER: 1967:38254 HCAPLUS
DOCUMENT ASSIGNEE(S): Santinflammatory and analgesic agents
KAMIN, Saul Bernard
FILE TICL, USA
EUR. Pat. Appl., 56 pp.
CODEN: EYKENDW
DOCUMENT TYPE: LANGUAGE: English
FAMILY ACC. NUM. COUNT: 9
PATENT INFORMATION:

PATENT INFORMATION:				
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 208510	A2	19870114	EP 1986-305144	19860702
EP 208510	A3	19880302	EP 1986-303144	19860/02
	B1			
EP 208510		19910911		
R: AT, BE, CH,			, LU, NL, SE	
US 4678802	A	19870707		19860131
AT 67185	Ε	19910915		19860702
CA 1286663	A1	19910723		19860707
DK 8603242	A	19870110	DK 1986-3242	19860708
FI 8602882	A	19870110	FI 1986-2882	19860708
NO 8602750	A	19870112	NO 1986-2750	19860708
JP 62026269	A2	19870204	JP 1986-160675	19860708
JP 06010193	В4	19940209		
AU 8659847	A1	19870409	AU 1986-59847	19860708
AU 566065	B2	19871008		
HU 41386	A2	19870428	HU 1986-2844	19860708
HU 198015	В	19890728		
ES 2001855	A6	19880701	ES 1986-191	19860708
IL 79356	A1	19900319	IL 1986-79356	19860708
CN 86105309	A	19870114	CN 1986-105309	19860709
ES 2009227	A6	19890916	ES 1987-3589	19871215
PRIORITY APPLN. INFO.:			US 1985-753200 A	19850709
			US 1986-821296 A	
			US 1986-825017 A	
			EP 1986-305144 A	
				

OTHER SOURCE(S): CASREACT 106:138254 IT 107315-25-3P 107315-36-6P 107315-56-0P

Page 5130/08/2005

LB ANSWER 39 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A , NO2

ANSWER 40 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)
107315-80-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as analgesic and antiinflammatory agent)
107315-25-3 HCAPLUS
1H-Indole-1,3-dicarboxamide, 2,3-dihydro-2-oxo-N3-2-thienyl- (9CI) (CA INDEX NAME)

107315-36-6 HCAPLUS 1H-Indole-1,3-dicarboxamide, 5-chloro-2,3-dihydro-2-oxo-N3-2-thienyl-(SCI) (CA INDEX NAME)

107315-56-0 HCAPLUS
1H-Indole-1,3-dicarboxamide, 2,3-dihydro-N1-(4-methoxyphenyl)-2-oxo-N3-2-thienyl-(9CI) (CA INDEX NAME)

107315-80-0 HCAPLUS
5H-1,3-Dioxolo[4,5-f]indole-5,7-dicarboxamide, 6,7-dihydro-N5-(4-

ANSWER 40 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) methoxyphenyl)-6-oxo-N7-2-thienyl- (9C1) (CA INDEX NAME)

ANSWER 41 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

77604-47-8P 77604-48-9P 77604-47-8P 77604-48-9P
RE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antiviral activity of)
77604-47-8 HCAPLUS
IH-Pytrole-2-carboxamide, N-[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pytrol-2-yl)1-1-methyl-5-[(1-methyl-5-nitro-IH-pytrol-2-yl)carbonyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

77604-48-9 HCAPLUS
1H-Pyrrole-2-carboxamide, N-(5-[((3-amino-3-iminopropyl)amino)carbonyl)-1-methyl-1H-pyrrol-2-yl)-5-[[(5-(formylamino)-1-methyl-1H-pyrrol-2-yl)carbonyl]amino)-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

• HC1

PAGE 1-B

77604-45-69
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and reduction-acylation reactions of) 77604-45-6 HCAPIUS

Page 5230/08/2005

ANSWER 41 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 12 May 1984

AB Distamycin A and congocidine isomers and homologs I (R = NO2, HCONH) and II [Rl = NO2, H2NC(:NH)NHCH2CONH] were prepared and their cytotoxicity tested. Thus, acylation of H2NCH2CH2CN by 1-methyl-5-nitro-2-pyrrolecarbonyl chloride gave the pyrrolycarboxamidopropionitrie III, which was treated with EtOH-HCl at O° for 1 h and then with NN3(g) to give II (Rl = NO2). I were obtained by successive acylation-reduction reactions of 1-methyl-5-nitro-2-carboxylic acid. II (Rl = NO2) possessed the highest antiviral activity in the series, and was less toxic and had the same antiviral activity as distamycin A. ACCESSION NUMEER: 1981:192034 HCAPLUS

DOCUMENT NUMBER: 34:192034 HCAPLUS

Structure-activity relationships of pyrrole amidine antiviral antibiotics. III: Preparation of distamycin and congocidine derivatives based on 2,5-disubstituted pyrroles

Becker, Yechiel

CORPORATE SOURCE: Becker, Yechiel

CORPORATE SOURCE: Pharm. Sch., Hebrew Univ., Jerusalem, Israel

Journal of Pharmaceutical Sciences (1980), 69(11), 134-8

CODEN: JPMSAE; ISSN: 0022-3549

DOCUMENT TYPE: June 1 of H2 propers of the property of th

Journal

English

DOCUMENT TYPE: LANGUAGE: IT 77604-46-7P

77604-46-7P
RE: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation); RACT (Reactant or reagent)
(preparation and aminolysis of, carboxamidemide derivative from)
77604-66-7 HCAPLUS
1H-Pyrrole-2-carboxamide, N-[5-[{(2-cyanoethyl)amino|carbonyl]-1-methyl-1H-pyrrol-2-yl)-1-methyl-5-{[(1-methyl-5-nitro-1H-pyrrol-2-yl)carbonyl]amino}(9CI) (CA INDEX NAME)

ANSWER 41 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 1H-Pyrrole-Z-carboxamide, N-[5-[[(2-cyanoethyl]>mino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-5-nitro-[9CI] (CA INDEX NAME)

77604-49-0P RL: SPN (Synthetic preparation); PREP (Preparation)

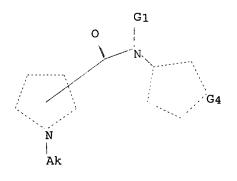
RE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
77604-49-0 HCAPLUS
H-Pyrrole-2-carboxamide, 5-{{5-{{(aminoiminomethyl)amino}acetyl}amino}1-methyl-1H-pyrrol-2-yl]carbonyl]aminoj-N-{5-{{(3-amino-3iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-,
dihydrochloride (9CI) (CA INDEX NAME)

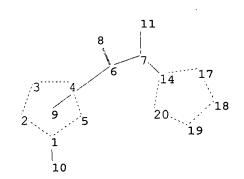
●2 HC1

PAGE 1-B

=> log y
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE
-29.93
-29.93

STN INTERNATIONAL LOGOFF AT 13:53:33 ON 30 AUG 2005





chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

 $1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 4-5 \quad 14-17 \quad 14-20 \quad 17-18 \quad 18-19 \quad 19-20$

exact/norm bonds :

 $1-2 \quad 1-5 \quad 1-10 \quad 2-3 \quad 3-4 \quad 4-5 \quad 6-7 \quad 6-8 \quad 7-11 \quad 7-14 \quad 14-17 \quad 14-20 \quad 17-18 \quad 18-19 \quad 19-20$

G1:H,CH3

G2:0,S

G3:0,N

G4:0,S,N

Match level :

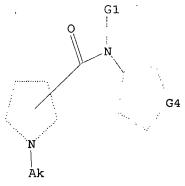
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 H, Me

G2 0, S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 17:24:33 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2836 TO ITERATE

70.5% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 53526 TO 59914

PROJECTED ANSWERS: 10740 TO 13706

L2 50 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 17:24:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 54653 TO ITERATE

100.0% PROCESSED 54653 ITERATIONS 11606 ANSWERS

SEARCH TIME: 00.00.04

L3 11606 SEA SSS FUL L1

=> fil hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL

FULL ESTIMATED COST ENTRY SESSION 161.76 161.97

FILE 'HCAPLUS' ENTERED AT 17:24:59 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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Page 430/08/2005

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FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13 L4 1844 L3

=> fil reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 2.45 164.42

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 17:25:13 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3 DICTIONARY FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

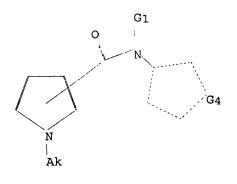
Please note that search-term pricing does apply when conducting SmartSELECT searches.

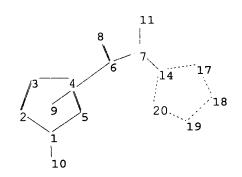
Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\exp3update.str

Page 530/08/2005





chain nodes :
6 7 8 10 11
ring nodes :
1 2 3 4 5 14 17 18 19 20
chain bonds :
1-10 6-7 6-8 7-11 7-14
ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

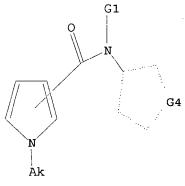
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L5 STRUCTURE UPLOADED

=> d 15 L5 HAS NO ANSWERS L5 STR



G1 H, Me

G2 O,S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 17:26:27 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2836 TO ITERATE

70.5% PROCESSED

2000 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

53526 TO 10553 TO 59914 13495

PROJECTED ANSWERS:

50 SEA SSS SAM L5

=> s 15 full

FULL SEARCH INITIATED 17:26:34 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 54653 TO ITERATE

100.0% PROCESSED

54653 ITERATIONS

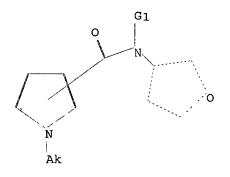
11202 ANSWERS

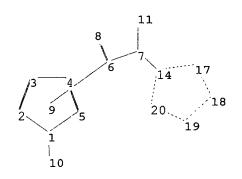
SEARCH TIME: 00.00.07

L7

11202 SEA SSS FUL L5

Uploading C:\Program Files\Stnexp\Queries\ppp.str





chain nodes :
6 7 8 10 11
ring nodes :
1 2 3 4 5 14 17 18 19 20
chain bonds :
1-10 6-7 6-8 7-11 7-14
ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

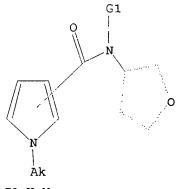
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L8 STRUCTURE UPLOADED

=> d 18 L8 HAS NO ANSWERS L8 STR



G1 H,Me

G2 0, S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 18

SAMPLE SEARCH INITIATED 17:28:03 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1636 TO ITERATE

100.0% PROCESSED 1

1636 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

30294 TO 35146

PROJECTED ANSWERS:

0 TO

Ь9

0 SEA SSS SAM L8

=> s 18 full

FULL SEARCH INITIATED 17:28:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 33735 TO ITERATE

100.0% PROCESSED 33735 ITERATIONS

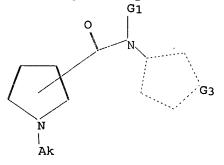
6 ANSWERS

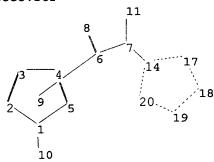
SEARCH TIME: 00.00.01

L10

6 SEA SSS FUL L8

=>
Uploading C:\Program Files\Stnexp\Queries\oooo.str





chain nodes : 6 7 8 10 11

ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

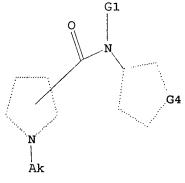
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L11 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Me

G2 0,S

G3 O, N

G4 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s 111

SAMPLE SEARCH INITIATED 17:29:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2664 TO ITERATE

Page 1030/08/2005

75.1% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 50185 TO 56375 PROJECTED ANSWERS: 10244 TO 13144

L12 50 SEA SSS SAM L11

=> fil hcaplus

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
325.67
490.09

50 ANSWERS

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FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 110

L13 1 L10

=> d ed abs ibib hitstr 113

ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 12 May 1984

H2CH (OR2) CH (CH2CHMe2) NHC (:X) CH (OR3) CH (OR4) CHR5CHR6COR7

CH (CH2CHMe2) NHC(:X) CH (OR3) CH (OH) CHR5CHR6COR7 II

AB Seven compds. with antiulcer activity, produced by Bacillus pumilus strain AI-77 during aerobic culture, have the structures I and II. These compds. also have antiinflammatory, anticholesteremic, antiarrhythmic, and vasodilatory activities and are intermediates for preparation of further compds. with these activities. For example, II-HCI (X = NH; R = R3 = R6 = H; R5 = NM2; R7 = OH) [77715-24-3] was produced by aerobic cultivation of B. pumilus AI-77 in 100 L defatted soybean meal-glucose-salts medium for 20 h at 30°, and was purified from the culture filtrate by chromatog, on Amberlite IRc-50 and XAD-2; the yield was 4.3 g. This compound at 50 mg/kg i.p. provided 100% protection against stress-induced ulcers in rats. The other 6 compds. were produced by B. pumilus in defatted soybean meal-corn steep liquor-sucrose-salts medium and separated by chromatog.

ACCESSION NUMBER: 1981:478461 HCAPLUS

1981:478461 HCAPLUS 95:78461 AI-77 compounds and their pharmaceutically acceptable salts DOCUMENT NUMBER: TITLE:

PATENT ASSIGNEE(S): SOURCE: Asahi Chemical Industry Co., Ltd., Japan Neth. Appl., 221 pp. CODEN: NAXXAN

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 8003985	A	19810113	NL 1980-3985	19800710
NL 187069	В	19901217		
NL 187069	С	19910516		
JP 56012352	A2	19810206	JP 1979-86892	19790711
JP 63034863	B4	19880712		
JP 56158778	A2	19811207	JP 1980-61685	19800512
JP 02046585	B4	19901016		

L13 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN

77676-14-3 HCAPLUS Hexonic acid, 2,3,6-trideoxy-6-[(1-{3,4-dihydro-8-hydroxy-1-oxo-1H-2-benzopyran-3-yl)-3-methylbutyl]amino]-3-[(11-methyl-1H-pyrrol-2-yl)carbonyl]amino]-6-oxo-, γ -lactone (9CI) (CA INDEX NAME)

77677-19-1 HCAPLUS
Hexonic acid, 3-[[[1-acetyl-lH-pyrrol-2-yl]carbonyl]amino]-2,3,6-trideoxy-6-[[1-[0-ethoxy-3,4-dihydro-1-oxo-1H-2-benzopyran-3-yl]-3-methylbutyl]amino]-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

77677-24-8 HCAPLUS
Hexonic acid, 3-[([1-acetyl-lH-indol-3-yl)carbonyl]amino]-2, 3, 6-trideoxy-6[(1-(8-ethoxy-3, 4-dihydro-1-oxo-1H-2-benzopyran-3-yl)-3-methylbutyl]amino]6-oxo-, y-lactone (9CI) (CA INDEX NAME)

(Continued) 19800704 19800708 DE 1980-3026214 19800710 19800710 19800711 19870507 JP 1987-109723 JP 1979-86892 JP 1980-61685 A 19790711 A 19800512

77676-13-2 HCAPLUS

Hexonic acid, 3-[[(1-acetyl-1H-pyrrol-2-yl)carbonyl)amino]-2,3,6-trideoxy-6-[[1-3,4-dihydro-8-hydroxy-1-oxo-1H-2-benzopyran-3-yl)-3-methylbutyl]amino]-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

L13 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN

77700-94-8 HCAPLUS

////00-94-8 HARPUS
Hexonic acid, 2.3,6-trideoxy-6-{{I-(8-ethoxy-3,4-dihydro-1-oxo-1H-2-benzopyran-3-yl)-3-methylbutyl|amino}-3-[{(1-methyl-1H-pyrrol-2-yl)carbonyl|amino}-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

=> fil reg COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	9.84	499.93
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.73	-0.73

FILE 'REGISTRY' ENTERED AT 17:31:41 ON 30 AUG 2005
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STRUCTURE FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3 DICTIONARY FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

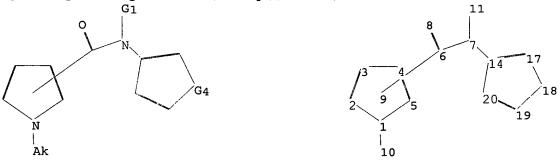
TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\nnn.str



chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

G4:0,S,N

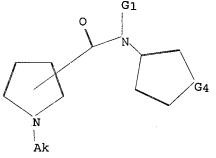
Match level :

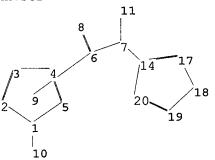
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L14 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\nnn.str





chain nodes :
6 7 8 10 11
ring nodes :
1 2 3 4 5 14 17 18 19 20
chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

 $1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 4-5 \quad 14-17 \quad 14-20 \quad 17-18 \quad 18-19 \quad 19-20$

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

G4:0,S,N

Match level :

Page 1430/08/2005

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L15 STRUCTURE UPLOADED

=> d 115 L15 HAS NO ANSWERS L15 STR

G1 H, Me

G2 0,S

G3 O,N

G4 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s 115

SAMPLE SEARCH INITIATED 17:33:09 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2836 TO ITERATE

70.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

53526 TO 59914

PROJECTED ANSWERS:

10420 TO 13344

L16

50 SEA SSS SAM L15

=> s 115 full

FULL SEARCH INITIATED 17:33:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 54653 TO ITERATE

100.0% PROCESSED 54653 ITERATIONS

11063 ANSWERS

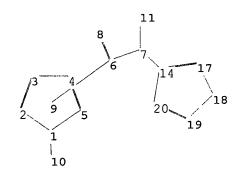
SEARCH TIME: 00.00.04

L17 11063 SEA SSS FUL L15

=>

Uploading C:\Program Files\Stnexp\Queries\yyyy.str

Page 1530/08/2005



chain nodes :
6 7 8 10 11
ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20 isolated ring systems :

containing 1 : 14 :

G1:H,CH3

G2:0,S

G3:0,N

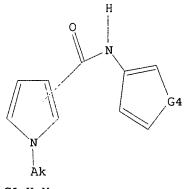
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L18 STRUCTURE UPLOADED

=> d 118 L18 HAS NO ANSWERS L18 STR



G1 H, Me

G2 O,S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 118

SAMPLE SEARCH INITIATED 17:35:14 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1019 TO ITERATE

100.0% PROCESSED

1019 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

18465 TO 22295 12980

PROJECTED ANSWERS:

10098 TO

L19

50 SEA SSS SAM L18

=> log y

SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION FULL ESTIMATED COST 163.48 663.41 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

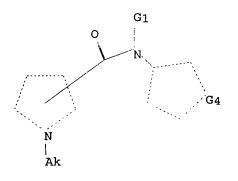
0.00 -0.73

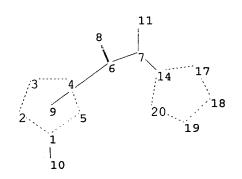
SESSION

ENTRY

CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 17:35:22 ON 30 AUG 2005





chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

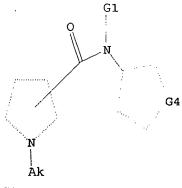
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G2 0,S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

50 ANSWERS

=> s 11

SAMPLE SEARCH INITIATED 17:24:33 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -2836 TO ITERATE

70.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 53526 TO 59914

PROJECTED ANSWERS: 10740 TO 13706

50 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 17:24:39 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 54653 TO ITERATE

100.0% PROCESSED 54653 ITERATIONS 11606 ANSWERS

SEARCH TIME: 00.00.04

11606 SEA SSS FUL L1 L3

=> fil hcaplus

SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION

161.97 FULL ESTIMATED COST 161.76

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FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3 L4 1844 L3

=> fil reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 2.45 164.42

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3 DICTIONARY FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

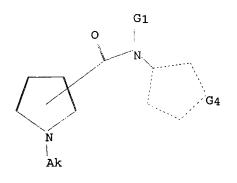
TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

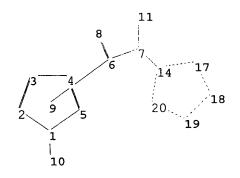
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\exp3update.str





chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

 $1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 4-5 \quad 14-17 \quad 14-20 \quad 17-18 \quad 18-19 \quad 19-20$

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

G4:0,S,N

Match level :

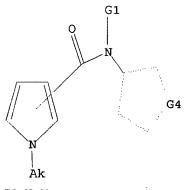
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



G2 0, S

G3 O,N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 17:26:27 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2836 TO ITERATE

70.5% PROCESSED

2000 ITERATIONS

BATCH

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE **COMPLETE** **COMPLETE**

PROJECTED ITERATIONS:

53526 TO 59914

PROJECTED ANSWERS:

10553 TO 13495

L6

50 SEA SSS SAM L5

=> s 15 full

FULL SEARCH INITIATED 17:26:34 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 54653 TO ITERATE

100.0% PROCESSED

54653 ITERATIONS

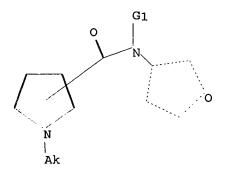
11202 ANSWERS

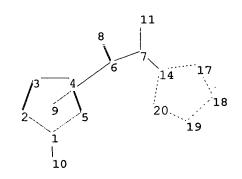
SEARCH TIME: 00.00.07

L7

11202 SEA SSS FUL L5

Uploading C:\Program Files\Stnexp\Queries\ppp.str





chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

 $1-2 \quad 1-5 \quad 1-10 \quad 2-3 \quad 3-4 \quad 4-5 \quad 6-7 \quad 6-8 \quad 7-11 \quad 7-14 \quad 14-17 \quad 14-20 \quad 17-18 \quad 18-19 \quad 19-20$

G1:H,CH3

G2:0,S

G3:0,N

G4:0,S,N

Match level :

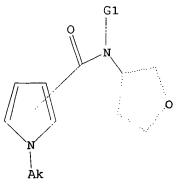
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 20:Atom

L8 STRUCTURE UPLOADED

=> d 18

L8 HAS NO ANSWERS

38 STR



G2 0,S

G3 O,N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 18

SAMPLE SEARCH INITIATED 17:28:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1636 TO ITERATE

100.0% PROCESSED

1636 ITERATIONS

0 ANSWERS

6 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE

BATCH **COMPLETE**

DAICH

PROJECTED ITERATIONS: 30294 TO 35146

PROJECTED ANSWERS:

0 TO

COMPLETE

L9 0 SEA SSS SAM L8

L10

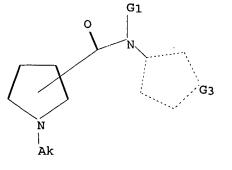
=> s 18 full FULL SEARCH INITIATED 17:28:10 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 33735 TO ITERATE

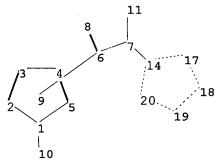
100.0% PROCESSED 33735 ITERATIONS

SEARCH TIME: 00.00.01

6 SEA SSS FUL L8

Uploading C:\Program Files\Stnexp\Queries\oooo.str





chain nodes:
6 7 8 10 11
ring nodes:

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H, CH3

G2:0,S

G3:0,N

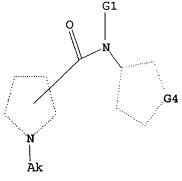
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L11 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Me

G2 0, S

G3 O, N

G4 0, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s l11

SAMPLE SEARCH INITIATED 17:29:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2664 TO ITERATE

Page 1030/08/2005

75.1% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

50 ANSWERS

PROJECTED ITERATIONS: 50185 TO 56375 PROJECTED ANSWERS: 10244 TO 13144

L12 50 SEA SSS SAM L11

=> fil hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL

FULL ESTIMATED COST ENTRY SESSION 325.67 490.09

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FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 110

L13 1 L10

=> d ed abs ibib hitstr 113

ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 12 May 1984

H2CH (OR2) CH (CH2CHMe2) NHC (:X) CH (OR3) CH (OR4) CHR5CHR6COR7

AB Seven compds. with antiulcer activity, produced by Bacillus pumilus strain AI-77 during aerobic culture, have the structures I and II. These compds. also have antiinflammatory, anticholesteremic, antiarrhythmic, and vasodilatory activities and are intermediates for preparation of further compds. With these activities. For example, II-Hcl (X = NH: R = R3 = R6 = H: R5 = NH2: R7 = OH) [7715-24-3] was produced by acrobic cultivation of B. pumilus AI-77 in 100 L defatted soybean meal-glucose-salts medium for 20 h at 30°, and was purified from the culture filtrate by chromatog, on Amberlite IRC-50 and XAD-2; the yield was 4.3 g. This compound at 50 mg/kg i.p. provided 100% protection against stress-induced ulcers in rats. The other 6 compds. were produced by B. pumilus in defatted soybean meal-corn steep liquor-sucrose-salts medium and separated by ACCESSION NUMBER: 1981:478461 HCAPLUS
DOCUMENT NUMBER: 95:78461
TITLE: AI-77 compounds and ****

1981:478461 HCAPLUS 95:78461 A1-77 compounds and their pharmaceutically acceptable salts Asahi Chemical Industry Co., Ltd., Japan Neth. Appl., 221 pp. CODEN: NAXXAN Patent

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 8003985	A	19810113	NL 1980-3985	19800710
NL '187069	В	19901217		
NL 187069	c	19910516		
JP 56012352	A2	19810206	JP 1979-86892	19790711
JP 63034863	B4	19880712		
JP 56158778	A2	19811207	JP 1980-61685	19800512
JP 02046585	84	19901016		

(Continued) L13 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN

77676-14-3 HCAPLUS
Hexonic acid, 2,3,6-trideoxy-6-[[1-{3,4-dihydro-8-hydroxy-1-oxo-1H-2-benzopyran-3-y1)-3-methylbutyl]amino]-3-[[(1-methyl-1H-pyrro1-2-y1)carbonyl]amino]-6-oxo-, y-lactone (SCI) (CA INDEX NAME)

77677-19-1 HCAPLUS
HEXONIC acid, 3-[{[1-acetyl-1H-pyrrol-2-yl]carbonyl]amino]-2,3,6-trideoxy-6-[[1-(8-ethoxy-3,4-dihydro-1-oxo-1H-2-benzopyran-3-yl]-3-methylbutyl]amino]-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

77677-24-8 HCAPLUS
Hexonic acid, 3-[([1-acetyl-1H-indol-3-yl)carbonyl]amino]-2,3,6-trideoxy-6[[1-(8-ethoxy-3,4-dihydro-1-oxo-1H-2-benzopyran-3-yl)-3-methylbutyl]amino]-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

19800704 19800708 DE 1980-3026214 19800710 CH 1980-5281 US 1980-167581 JP 1987-109723 19800710 19800711 19870507 PRIORITY APPLN. INFO.: JP 1979-86892 JP 1980-61685 A 19790711 A 19800512

//BJD-13-2 MOMPHUS Hexonic acid, 3-[[(1-acetyl-1H-pyrrol-2-yl)carbonyl]amino]-2,3,6-trideoxy-6-[[1-(3,4-dl)dro-8-hydroxy-1-oxo-1H-2-benzoypara-3-yl)-3-methylbutyl amino]-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

(Continued) L13 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN

77700-94-8 HCAPLUS
Hexonic acid, 2,3,6-trideoxy-6-{[1-(8-ethoxy-3,4-dihydro-1-oxo-1H-2-benzopyran-3-y1)-3-methylbutyl]amino]-3-[[(1-methyl-1H-pyrrol-2-y1)carbonyl]amino]-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	9.84	499.93
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.73	-0.73

FILE 'REGISTRY' ENTERED AT 17:31:41 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3 DICTIONARY FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

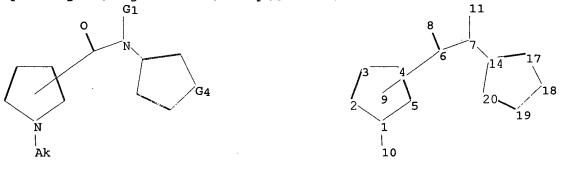
TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> Uploading C:\Program Files\Stnexp\Queries\nnn.str



chain nodes :
6 7 8 10 11
ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H, CH3

G2:0,S

G3:0,N

G4:0,S,N

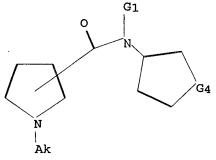
Match level:

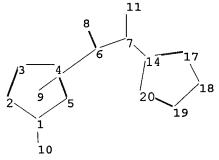
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L14 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\nnn.str





chain nodes : 6 7 8 10 11 ring nodes :

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

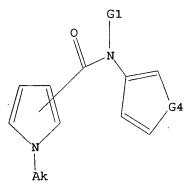
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L15 STRUCTURE UPLOADED

=> d 115 L15 HAS NO ANSWERS L15 STR



G1 H,Me

G2 0,S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

50 ANSWERS

=> s 115

SAMPLE SEARCH INITIATED 17:33:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2836 TO ITERATE

70.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 53526 TO 59914
PROJECTED ANSWERS: 10420 TO 13344

L16 50 SEA SSS SAM L15

=> s 115 full

FULL SEARCH INITIATED 17:33:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 54653 TO ITERATE

100.0% PROCESSED 54653 ITERATIONS 11063 ANSWERS SEARCH TIME: 00.00.04

L17 11063 SEA SSS FUL L15

Uploading C:\Program Files\Stnexp\Queries\yyyy.str

Page 1530/08/2005

chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

 $1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 4-5 \quad 14-17 \quad 14-20 \quad 17-18 \quad 18-19 \quad 19-20$

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

isolated ring systems :

containing 1 : 14 :

G1:H,CH3

G2:0,S

G3:0,N

G4:0,S,N

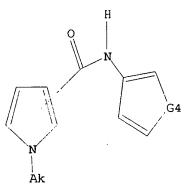
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L18 STRUCTURE UPLOADED

=> d 118 L18 HAS NO ANSWERS L18 STR

The second of th



G2 0, S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 118

SAMPLE SEARCH INITIATED 17:35:14 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1019 TO ITERATE

100.0% PROCESSED

1019 ITERATIONS

50 ANSWERS

-0.73

0.00

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

22295

PROJECTED ITERATIONS:

CA SUBSCRIBER PRICE

18465 TO 12980

PROJECTED ANSWERS:

10098 TO

L19

50 SEA SSS SAM L18

=> log y

SINCE FILE TOTAL COST IN U.S. DOLLARS SESSION ENTRY FULL ESTIMATED COST 163.48 663.41 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

STN INTERNATIONAL LOGOFF AT 17:35:22 ON 30 AUG 2005